SECTION 1
ORGANIC COMPOUNDS

1.1 NOMENCLATURE OF ORGANIC COMPOUNDS

The following synopsis of rules for naming organic compounds and the examples given in explanation are not intended to cover all the possible cases. For a more comprehensive and detailed description, see J. Rigaudy and S. P. Klesney, *Nomenclature of Organic Chemistry*, Sections A, B, C, D, E, F, and H, Pergamon Press, Oxford, 1979. This publication contains the recommendations of the Commission on Nomenclature of Organic Chemistry and was prepared under the auspices of the International Union of Pure and Applied Chemistry (IUPAC).

1.1.1 Nonfunctional Compounds

1.1.1.1 Alkanes. The saturated open-chain (acyclic) hydrocarbons (C_nH_{2n+2}) have names ending in -ane. The first four members have the trivial names *methane* (CH_4), *ethane* (CH_3CH_3 or C_2H_6), *propane* (C_3H_8), and *butane* (C_4H_{10}). For the remainder of the alkanes, the first portion of the name

is derived from the Greek prefix (see Table 2.4) that cites the number of carbons in the alkane followed by -ane with elision of the terminal -a from the prefix, as shown in Table 1.1.

TABLE 1.1 Names of Straight-Chain Alkanes

*n**	Name	*n**	Name	*n**	Name	*n**	Name
1	Methane	11	Undecane‡	21	Henicosane	60	Hexacontane
2	Ethane	12	Dodecane	22	Docosane	70	Heptacontane
3	Propane	13	Tridecane	23	Tricosane	80	Octacontane
4	Butane	14	Tetradecane			90	Nonacontane
5	Pentane	15	Pentadecane	30	Triacontane	100	Hectane
6	Hexane	16	Hexadecane	31	Hentriacontane	110	Decahectane
7	Heptane	17	Heptadecane	32	Dotriacontane	120	Icosahectane
8	Octane	18	Octadecane			121	Henicosahectane
9	Nonane†	19	Nonadecane	40	Tetracontane		
10	Decane	20	Icosane§	50	Pentacontane		

* n = total number of carbon atoms.
† Formerly called enneane.
‡ Formerly called hendecane.
§ Formerly called eicosane.

For branching compounds, the parent structure is the longest continuous chain present in the compound. Consider the compound to have been derived from this structure by replacement of hydrogen by various alkyl groups. Arabic number prefixes indicate the carbon to which the alkyl group is attached. Start numbering at whichever end of the parent structure that results in the lowest-numbered locants. The arabic prefixes are listed in numerical sequence, separated from each other by commas and from the remainder of the name by a hyphen.

If the same alkyl group occurs more than once as a side chain, this is indicated by the prefixes di-, tri-, tetra-, etc. Side chains are cited in alphabetical order (before insertion of any multiplying prefix). The name of a complex radical (side chain) is considered to begin with the first letter of its complete name. Where names of complex radicals are composed of identical words, priority for citation is given to that radical which contains the lowest-numbered locant at the first cited point of difference in the radical. If two or more side chains are in equivalent positions, the one to be assigned the lowest-numbered locant is that cited first in the name. The complete expression for the side chain may be enclosed in parentheses for clarity or the carbon atoms in side chains may be indicated by primed locants.

If hydrocarbon chains of equal length are competing for selection as the parent, the choice goes in descending order to (1) the chain that has the greatest number of side chains, (2) the chain whose side chains have the lowest-numbered locants, (3) the chain having the greatest number of carbon atoms in the smaller side chains, or (4) the chain having the least-branched side chains.

These trivial names may be used for the unsubstituted hydrocarbon only:

Isobutane $(CH_3)_2CHCH_3$ Neopentane $(CH_3)_4C$

Isopentane $(CH_3)_2CHCH_2CH_3$ Isohexane $(CH_3)_2CHCH_2CH_2CH_3$

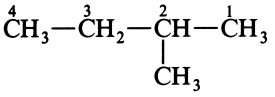
Univalent radicals derived from saturated unbranched alkanes by removal of hydrogen from a terminal carbon atom are named by adding -yl in place of -ane to the stem name. Thus the alkane

ethane becomes the radical *ethyl*. These exceptions are permitted for unsubstituted radicals only:

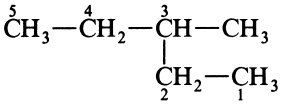
Isopropyl	$(CH_3)_2CH—$	Isopentyl	$(CH_3)_2CHCH_2CH_2—$
Isobutyl	$(CH_3)_2CHCH_2—$	Neopentyl	$(CH_3)_3CCH_2—$
sec-Butyl	$CH_3CH_2CH(CH_3)—$	*tert*-Pentyl	$CH_3CH_2C(CH_3)_2—$
tert-Butyl	$(CH_3)_3C—$	Isohexyl	$(CH_3)_2CHCH_2CH_2CH_2—$

Note the usage of the prefixes iso-, neo-, *sec*-, and *tert*-, and note when italics are employed. Italicized prefixes are never involved in alphabetization, except among themselves; thus *sec*-butyl would precede isobutyl, isohexyl would precede isopropyl, and *sec*-butyl would precede *tert*-butyl.

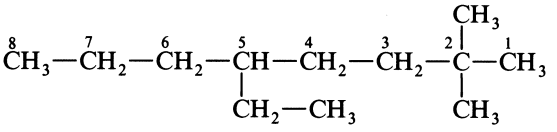
Examples of alkane nomenclature are



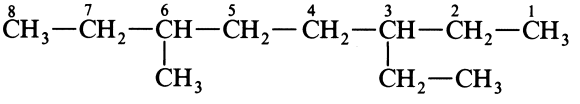
2-Methylbutane (or the trivial name, isopentane)



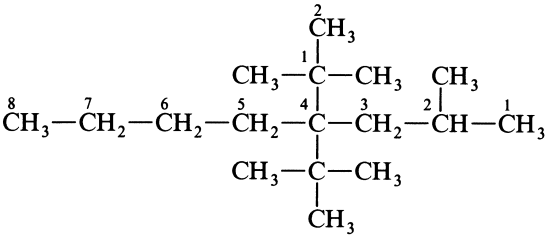
3-Methylpentane (not 2-ethylbutane)



5-Ethyl-2,2-dimethyloctane (note cited order)



3-Ethyl-6-methyloctane (note locants reversed)



4,4-Bis(1,1-dimethylethyl)-2-methyloctane
4,4-Bis-1′,1′-dimethylethyl-2-methyloctane
4,4-Bis(*tert*-butyl)-2-methyloctane

Bivalent radicals derived from saturated unbranched alkanes by removal of two hydrogen atoms are named as follows: (1) If both free bonds are on the same carbon atom, the ending -ane of the hydrocarbon is replaced with -ylidene. However, for the first member of the alkanes it is methylene

rather than methylidene. Isopropylidene, *sec*-butylidene, and neopentylidene may be used for the unsubstituted group only. (2) If the two free bonds are on different carbon atoms, the straight-chain group terminating in these two carbon atoms is named by citing the number of methylene groups comprising the chain. Other carbon groups are named as substituents. Ethylene is used rather than dimethylene for the first member of the series, and propylene is retained for $CH_3—\underset{|}{CH}—CH_2—$ (but trimethylene is $—CH_2—CH_2—CH_2—$).

Trivalent groups derived by the removal of three hydrogen atoms from the same carbon are named by replacing the ending -ane of the parent hydrocarbon with -ylidyne.

1.1.1.2 Alkenes and Alkynes. Each name of the corresponding saturated hydrocarbon is converted to the corresponding alkene by changing the ending -ane to -ene. For alkynes the ending is -yne. With more than one double (or triple) bond, the endings are -adiene, -atriene, etc. (or -adiyne, -atriyne, etc.). The position of the double (or triple) bond in the parent chain is indicated by a locant obtained by numbering from the end of the chain nearest the double (or triple) bond; thus $CH_3CH_2CH{=}CH_2$ is 1-butene and $CH_3C{\equiv}CCH_3$ is 2-butyne.

For multiple unsaturated bonds, the chain is so numbered as to give the lowest possible locants to the unsaturated bonds. When there is a choice in numbering, the double bonds are given the lowest locants, and the alkene is cited before the alkyne where both occur in the name. Examples:

$CH_3CH_2CH_2CH_2CH{=}CH—CH{=}CH_2$ 1,3-Octadiene

$CH_2{=}CHC{\equiv}CCH{=}CH_2$ 1,5-Hexadiene-3-yne

$CH_3CH{=}CHCH_2C{\equiv}CH$ 4-Hexen-1-yne

$CH{\equiv}CCH_2CH{=}CH_2$ 1-Penten-4-yne

Unsaturated branched acyclic hydrocarbons are named as derivatives of the chain that contains the maximum number of double and/or triple bonds. When a choice exists, priority goes in sequence to (1) the chain with the greatest number of carbon atoms and (2) the chain containing the maximum number of double bonds.

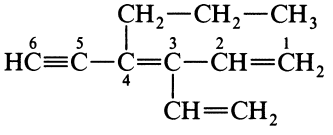
These nonsystematic names are retained:

Ethylene $CH_2{=}CH_2$

Allene $CH_2{=}C{=}CH_2$

Acetylene $HC{\equiv}CH$

An example of nomenclature for alkenes and alkynes is



4-Propyl-3-vinyl-1,3-hexadien-5-yne

Univalent radicals have the endings -enyl, -ynyl, -dienyl, -diynyl, etc. When necessary, the positions of the double and triple bonds are indicated by locants, with the carbon atom with the free valence numbered as 1. Examples:

$CH_2{=}CH—CH_2—$ 2-Propenyl

$CH_3—C{\equiv}C—$ 1-Propynyl

$CH_3—C{\equiv}C—CH_2CH{=}CH_2—$ 1-Hexen-4-ynyl

These names are retained:

Vinyl (for ethenyl) $CH_2{=}CH{-}$

Allyl (for 2-propenyl) $CH_2{=}CH{-}CH_2{-}$

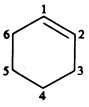
Isopropenyl (for 1-methylvinyl but for unsubstituted radical only) $CH_2{=}C(CH_3){-}$

Should there be a choice for the fundamental straight chain of a radical, that chain is selected which contains (1) the maximum number of double and triple bonds, (2) the largest number of carbon atoms, and (3) the largest number of double bonds. These are in descending priority.

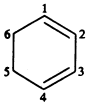
Bivalent radicals derived from unbranched alkenes, alkadienes, and alkynes by removing a hydrogen atom from each of the terminal carbon atoms are named by replacing the endings -ene, -diene, and -yne by -enylene, -dienylene, and -ynylene, respectively. Positions of double and triple bonds are indicated by numbers when necessary. The name *vinylene* instead of ethenylene is retained for $-CH{=}CH-$.

1.1.1.3 Monocyclic Aliphatic Hydrocarbons. Monocyclic aliphatic hydrocarbons (with no side chains) are named by prefixing cyclo- to the name of the corresponding open-chain hydrocarbon having the same number of carbon atoms as the ring. Radicals are formed as with the alkanes, alkenes, and alkynes. Examples:

Cyclohexane — Cyclohexyl- (for the radical)



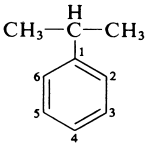
Cyclohexene — 1-Cyclohexenyl- (for the radical with the free valence at carbon 1)



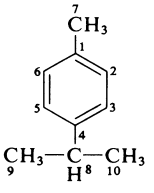
1,3-Cyclohexandiene — Cyclohexadienyl- (the unsaturated carbons are given numbers as low as possible, numbering from the carbon atom with the free valence given the number 1)

For convenience, aliphatic rings are often represented by simple geometric figures: a triangle for cyclopropane, a square for cyclobutane, a pentagon for cyclopentane, a hexagon (as illustrated) for cyclohexane, etc. It is understood that two hydrogen atoms are located at each corner of the figure unless some other group is indicated for one or both.

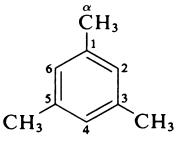
1.1.1.4 Monocyclic Aromatic Compounds. Except for six retained names, all monocyclic substituted aromatic hydrocarbons are named systematically as derivatives of benzene. Moreover, if the substituent introduced into a compound with a retained trivial name is identical with one already present in that compound, the compound is named as a derivative of benzene. These names are retained:



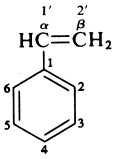
Cumene



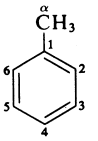
Cymene (all three forms; *para*- shown)



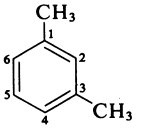
Mesitylene



Styrene



Toluene



Xylene (all three forms; *meta*- shown)

The position of substituents is indicated by numbers, with the lowest locant possible given to substituents. When a name is based on a recognized trivial name, priority for lowest-numbered locants is given to substituents implied by the trivial name. When only two substituents are present on a benzene ring, their position may be indicated by *o*- (*ortho*-), *m*- (*meta*-), and *p*- (*para*-) (and alphabetized in the order given) used in place of 1,2-, 1,3-, and 1,4-, respectively.

Radicals derived from monocyclic substituted aromatic hydrocarbons and having the free valence at a ring atom (numbered 1) are named phenyl (for benzene as parent, since benzyl is used for the radical $C_6H_5CH_2$—), cumenyl, mesityl, tolyl, and xylyl. All other radicals are named as substituted phenyl radicals. For radicals having a single free valence in the side chain, these trivial names are retained:

Benzyl $C_6H_5CH_2$—

Benzhydryl (alternative to diphenylmethyl) $(C_6H_5)_2CH$—

Cinnamyl $C_6H_5CH{=}CH{-}CH_2$—

Phenethyl $C_6H_5CH_2CH_2$—

Styryl $C_6H_5CH{=}CH$—

Trityl $(C_6H_5)_3C$—

Otherwise, radicals having the free valence(s) in the side chain are named in accordance with the rules for alkanes, alkenes, or alkynes.

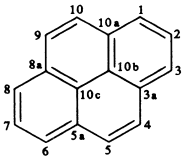
The name *phenylene* (*o*-, *m*-, or *p*-) is retained for the radical —C_6H_4—. Bivalent radicals formed from substituted benzene derivatives and having the free valences at ring atoms are named as substituted phenylene radicals, with the carbon atoms having the free valences being numbered 1,2-, 1,3-, or 1,4-, as appropriate.

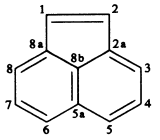
Radicals having three or more free valences are named by adding the suffixes -triyl, -tetrayl, etc. to the systematic name of the corresponding hydrocarbon.

1.1.1.5 Fused Polycyclic Hydrocarbons. The names of polycyclic hydrocarbons containing the maximum number of conjugated double bonds end in -ene. Here the ending does not denote one double bond. Names of hydrocarbons containing five or more fixed benzene rings in a linear arrangement are formed from a numerical prefix (see Table 2.4) followed by -acene. A partial list of the names of polycyclic hydrocarbons is given in Table 1.2. Many names are trivial.

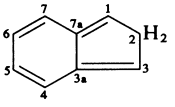
Numbering of each ring system is fixed, as shown in Table 1.2, but it follows a systematic pattern. The individual rings of each system are oriented so that the greatest number of rings are (1) in a horizontal row and (2) the maximum number of rings are above and to the right (upper-right quadrant) of the horizontal row. When two orientations meet these requirements, the one is chosen that has the fewest rings in the lower-left quadrant. Numbering proceeds in a clockwise direction, commencing with the carbon atom not engaged in ring fusion that lies in the most counterclockwise position of the uppermost ring (upper-right quadrant); omit atoms common to two or more rings. Atoms common to two or more rings are designated by adding lowercase roman letters to the number of the position immediately preceding. Interior atoms follow the highest number, taking a clockwise

sequence wherever there is a choice. Anthracene and phenanthrene are two exceptions to the rule on numbering. Two examples of numbering follow:

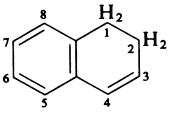




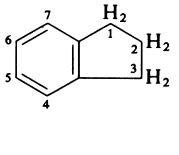
When a ring system with the maximum number of conjugated double bonds can exist in two or more forms differing only in the position of an "extra" hydrogen atom, the name can be made specific by indicating the position of the extra hydrogen(s). The compound name is modified with a locant followed by an italic capital *H* for each of these hydrogen atoms. Carbon atoms that carry an indicated hydrogen atom are numbered as low as possible. For example, 1*H*-indene is illustrated in Table 1.2; 2*H*-indene would be



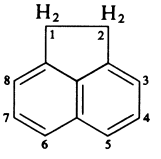
Names of polycyclic hydrocarbons with less than the maximum number of noncumulative double bonds are formed from a prefix dihydro-, tetrahydro-, etc., followed by the name of the corresponding unreduced hydrocarbon. The prefix perhydro- signifies full hydrogenation. For example, 1,2-dihydronaphthalene is



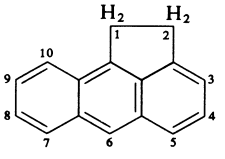
Examples of retained names and their structures are as follows:



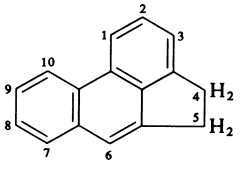
Indan



Acenaphthene



Aceanthrene



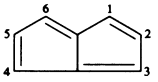
Acephenanthrene

Polycyclic compounds in which two rings have two atoms in common or in which one ring contains two atoms in common with each of two or more rings of a contiguous series of rings and which contain at least two rings of five or more members with the maximum number of noncumu-

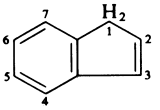
TABLE 1.2 Fused Polycyclic Hydrocarbons

Listed in order of increasing priority for selection as parent compound.

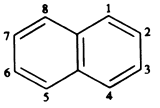
1. Pentalene



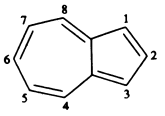
2. Indene



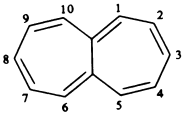
3. Naphthalene



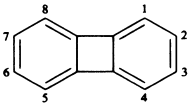
4. Azulene



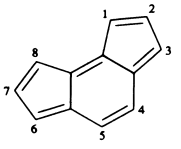
5. Heptalene



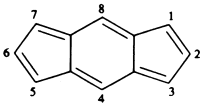
6. Biphenylene



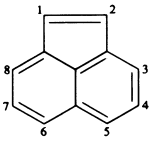
7. *asym*-Indacene



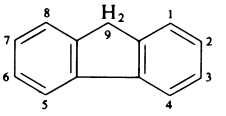
8. *sym*-Indacene



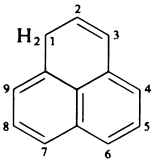
9. Acenaphthylene



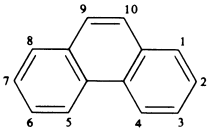
10. Fluorene



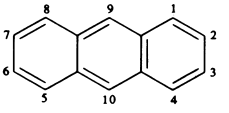
11. Phenalene



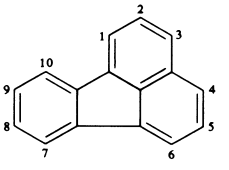
12. Phenanthrene*



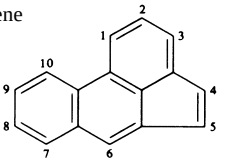
13. Anthracene*



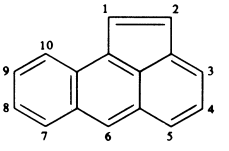
14. Fluoranthene



15. Acephenanthrylene

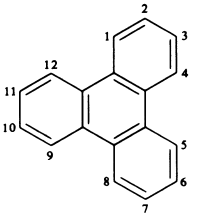
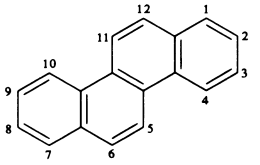
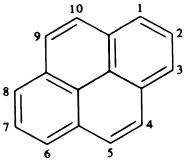
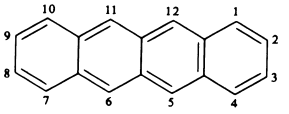


16. Aceanthrylene



* Asterisk after a compound denotes exception to systematic numbering.

TABLE 1.2 Fused Polycyclic Hydrocarbons (*Continued*)

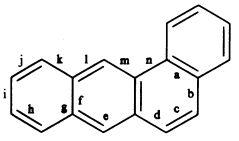
17. Triphenylene 	19. Chrysene 
18. Pyrene 	20. Naphthacene 

lative double bonds and which have no accepted trivial name (Table 1.2) are named by prefixing to the name of the parent ring or ring system designations of the other components. The parent name should contain as many rings as possible (provided it has a trivial name) and should occur as far as possible from the beginning of the list in Table 1.2. Furthermore, the attached component(s) should be as simple as possible. For example, one writes dibenzophenanthrene and not naphthophenanthrene because the attached component benzo- is simpler than napththo-. Prefixes designating attached components are formed by changing the ending -ene into -eno-; for example, indeno- from indene. Multiple prefixes are arranged in alphabetical order. Several abbreviated prefixes are recognized; the parent is given in parentheses:

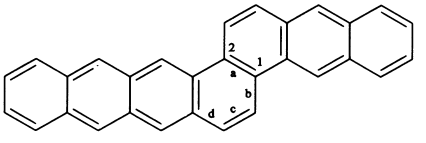
Acenaphtho-	(acenaphthylene)	Naphtho-	(naphthalene)
Anthra-	(anthracene)	Perylo-	(perylene)
Benzo-	(benzene)	Phenanthro-	(phenanthrene)

For monocyclic prefixes other than benzo-, the following names are recognized, each to represent the form with the maximum number of noncumulative double bonds: cyclopenta-, cyclohepta-, cycloocta-, etc.

Isomers are distinguished by lettering the peripheral sides of the parent beginning with *a* for the side 1,2, and so on, lettering every side around the periphery. If necessary for clarity, the numbers of the attached position (1,2, for example) of the substituent ring are also denoted. The prefixes are cited in alphabetical order. The numbers and letters are enclosed in square brackets and placed immediately after the designation of the attached component. Examples are

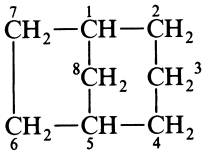


Benz[α]anthracene

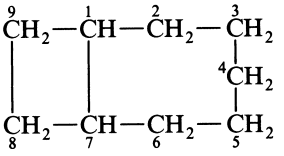


Anthra[2,1-α]naphthacene

1.1.1.6 Bridged Hydrocarbons. Saturated alicyclic hydrocarbon systems consisting of two rings that have two or more atoms in common take the name of the open-chain hydrocarbon containing the same total number of carbon atoms and are preceded by the prefix bicyclo-. The system is numbered commencing with one of the bridgeheads, numbering proceeding by the longest possible path to the second bridgehead. Numbering is then continued from this atom by the longer remaining unnumbered path back to the first bridgehead and is completed by the shortest path from the atom next to the first bridgehead. When a choice in numbering exists, unsaturation is given the lowest numbers. The number of carbon atoms in each of the bridges connecting the bridgeheads is indicated in brackets in descending order. Examples are

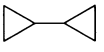


Bicyclo[3.2.1]octane

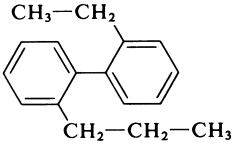


Bicyclo[5.2.0]nonane

1.1.1.7 Hydrocarbon Ring Assemblies. Assemblies are two or more cyclic systems, either single rings or fused systems, that are joined directly to each other by double or single bonds. For identical systems naming may proceed (1) by placing the prefix bi- before the name of the corresponding radical or (2), for systems joined through a single bond, by placing the prefix bi- before the name of the corresponding hydrocarbon. In each case, the numbering of the assembly is that of the corresponding radical or hydrocarbon, one system being assigned unprimed numbers and the other primed numbers. The points of attachment are indicated by placing the appropriate locants before the name; an unprimed number is considered lower than the same number primed. The name *biphenyl* is used for the assembly consisting of two benzene rings. Examples are



1,1′-Bicyclopropyl or 1,1′-bicyclopropane



2-Ethyl-2′-propylbiphenyl

For nonidentical ring systems, one ring system is selected as the parent and the other systems are considered as substituents and are arranged in alphabetical order. The parent ring system is assigned unprimed numbers. The parent is chosen by considering the following characteristics in turn until a decision is reached: (1) the system containing the larger number of rings, (2) the system containing the larger ring, (3) the system in the lowest state of hydrogenation, and (4) the highest-order number of ring systems set forth in Table 1.2. Examples are given, with the deciding priority given in parentheses preceding the name:

(1) 2-Phenylnaphthalene

(2) and (4) 2-(2′-Naphthyl)azulene

(3) Cyclohexylbenzene

1.1.1.8 Radicals from Ring Systems. Univalent substituent groups derived from polycyclic hydrocarbons are named by changing the final *e* of the hydrocarbon name to -yl. The carbon atoms having free valences are given locants as low as possible consistent with the fixed numbering of the

hydrocarbon. Exceptions are naphthyl (instead of naphthalenyl), anthryl (for anthracenyl), and phenanthryl (for phenanthrenyl). However, these abbreviated forms are used only for the simple ring systems. Substituting groups derived from fused derivatives of these ring systems are named systematically. Substituting groups having two or more free bonds are named as described in Monocyclic Aliphatic Hydrocarbons on p. 1.5.

1.1.1.9 Cyclic Hydrocarbons with Side Chains. Hydrocarbons composed of cyclic and aliphatic chains are named in a manner that is the simplest permissible or the most appropriate for the chemical intent. Hydrocarbons containing several chains attached to one cyclic nucleus are generally named as derivatives of the cyclic compound, and compounds containing several side chains and/or cyclic radicals attached to one chain are named as derivatives of the acyclic compound. Examples are

2-Ethyl-1-methylnaphthalene

Diphenylmethane

1,5-Diphenylpentane

2,3-Dimethyl-1-phenyl-1-hexene

Recognized trivial names for composite radicals are used if they lead to simplifications in naming. Examples are

1-Benzylnaphthalene

1,2,4-Tris(3-*p*-tolylpropyl)benzene

Fulvene, for methylenecyclopentadiene, and stilbene, for 1,2-diphenylethylene, are trivial names that are retained.

1.1.1.10 Heterocyclic Systems. Heterocyclic compounds can be named by relating them to the corresponding carbocyclic ring systems by using replacement nomenclature. Heteroatoms are denoted by prefixes ending in *a*, as shown in Table 1.3. If two or more replacement prefixes are required in a single name, they are cited in the order of their listing in the table. The lowest possible numbers consistent with the numbering of the corresponding carbocyclic system are assigned to the heteroatoms and then to carbon atoms bearing double or triple bonds. Locants are cited immediately preceding the prefixes or suffixes to which they refer. Multiplicity of the same heteroatom is indicated by the appropriate prefix in the series: di-, tri-, tetra-, penta-, hexa-, etc.

TABLE 1.3 Specialist Nomenclature for Heterocyclic Systems

Heterocyclic atoms are listed in decreasing order of priority.

Element	Valence	Prefix	Element	Valence	Prefix
Oxygen	2	Oxa-	Antimony	3	Stiba-*
Sulfur	2	Thia-	Bismuth	3	Bisma-
Selenium	2	Selena-	Silicon	4	Sila-
Tellurium	2	Tellura-	Germanium	4	Germa-
Nitrogen	3	Aza-	Tin	4	Stanna-
Phosphorus	3	Phospha-*	Lead	4	Plumba-
Arsenic	3	Arsa-*	Boron	3	Bora-
			Mercury	2	Mercura-

* When immediately followed by -in or -ine, phospha- should be replaced by phosphor-, arsa- by arsen-, and stiba- by antimon-. The saturated six-membered rings corresponding to phosphorin and arsenin are named *phosphorinane* and *arsenane.* A further exception is the replacement of borin by borinane.

TABLE 1.4 Suffixes for Specialist Nomenclature of Heterocyclic Systems

Number of ring members	Rings containing nitrogen		Rings containing no nitrogen	
	Unsaturation*	Saturation	Unsaturation*	Saturation
3	-irine	-iridine	-irene	-irane
4	-ete	-etidine	-ete	-etane
5	-ole	-olidine	-ole	-olane
6	-ine†	‡	-in	-ane§
7	-epine	‡	-epin	-epane
8	-ocine	‡	-ocin	-ocane
9	-onine	‡	-onin	-onane
10	-ecine	‡	-ecin	-ecane

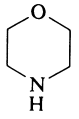
* Unsaturation corresponding to the maximum number of noncumulative double bonds. Heteroatoms have the normal valences given in Table 1.3.

† For phosphorus, arsenic, antimony, and boron, see the special provisions in Table 1.3.

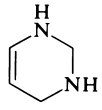
‡ Expressed by prefixing perhydro- to the name of the corresponding unsaturated compound.

§ Not applicable to silicon, germanium, tin, and lead; perhydro- is prefixed to the name of the corresponding unsaturated compound.

If the corresponding carbocyclic system is partially or completely hydrogenated, the additional hydrogen is cited using the appropriate *H*- or hydro- prefixes. A trivial name from Tables 1.5 and 1.6, if available, along with the state of hydrogenation may be used. In the specialist nomenclature for heterocyclic systems, the prefix or prefixes from Table 1.3 are combined with the appropriate stem from Table 1.4, eliding an *a* where necessary. Examples of acceptable usage, including (1) replacement and (2) specialist nomenclature, are



(1) 1-Oxa-4-azacyclohexane
(2) 1,4-Oxazoline
Morpholine



(1) 1,3-Diazacyclohex-5-ene
(2) 1,2,3,4-Tetrahydro-1,3-diazine

(1) Thiacyclopropane
(2) Thiirane
Ethylene sulfide

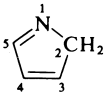
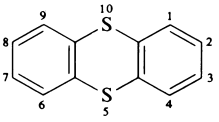
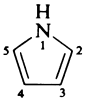
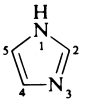
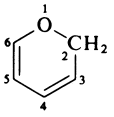
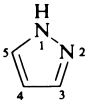
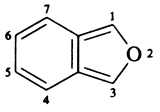
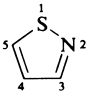
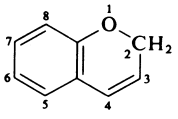
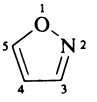
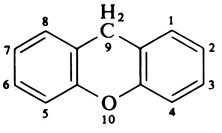
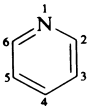
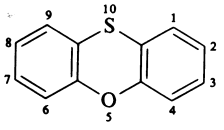
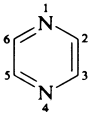
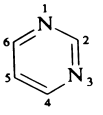
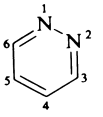
Radicals derived from heterocyclic compounds by removal of hydrogen from a ring are named by adding -yl to the names of the parent compounds (with elision of the final *e*, if present). These exceptions are retained:

Furyl (from furan)
Pyridyl (from pyridine)
Piperidyl (from piperidine)
Quinolyl (from quinoline)
Isoquinolyl
Thenylidene (for thienylmethylene)
Furfuryl (for 2-furylmethyl)
Furfurylidene (for 2-furylmethylene)
Thienyl (from thiophene)
Thenylidyne (for thienylmethylidyne)
Furfurylidyne (for 2-furylmethylidyne)
Thenyl (for thienylmethyl)

Also, piperidino- and morpholino- are preferred to 1-piperidyl- and 4-morpholinyl-, respectively.

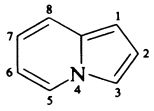
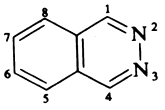
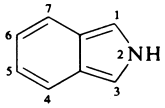
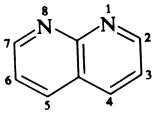
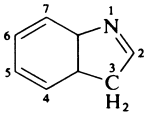
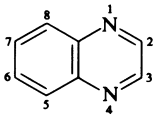
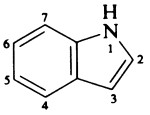
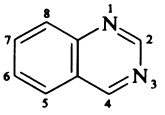
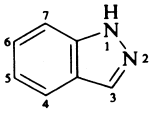
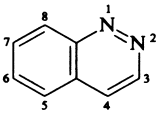
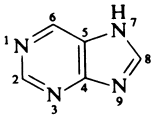
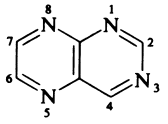
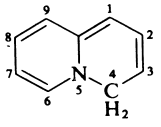
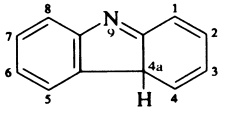
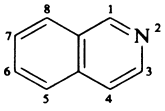
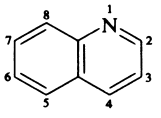
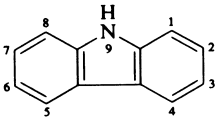
TABLE 1.5 Trivial Names of Heterocyclic Systems Suitable for Use in Fusion Names

Listed in order of increasing priority as senior ring system.

Structure	Parent name	Radical name	Structure	Parent name	Radical name
	Thiophene	Thienyl		2*H*-Pyrrole	2*H*-Pyrrolyl
	Thianthrene	Thianthrenyl		Pyrrole	Pyrrolyl
	Furan	Furyl		Imidazole	Imidazolyl
	Pyran (2*H*-shown)	Pyranyl		Pyrazole	Pyrazolyl
	Isobenzofuran	Isobenzo-furanyl		Isothiazole	Isothiazolyl
	Chromene (2*H*-shown)	Chromenyl		Isoxazole	Isoxazolyl
	Xanthene*	Xanthenyl		Pyridine	Pyridyl
	Phenoxathiin	Phenoxa-thiinyl		Pyrazine	Pyrazinyl
				Pyrimidine	Pyrimidinyl
				Pyridazine	Pyridazinyl

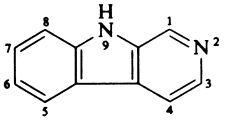
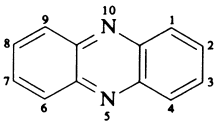
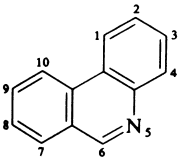
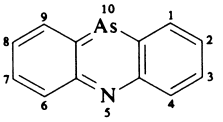
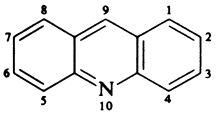
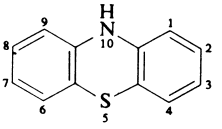
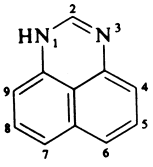
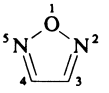
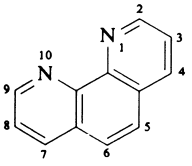
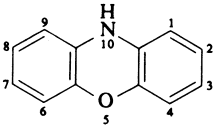
* Asterisk after a compound denotes exception to systematic numbering.

TABLE 1.5 Trivial Names of Heterocyclic Systems Suitable for Use in Fusion Names (*Continued*)

Structure	Parent name	Radical name	Structure	Parent name	Radical name
	Indolizine	Indolizinyl		Phthalazine	Phthalazinyl
	Isoindole	Isoindolyl		Naphthyridine (1,8-shown)	Naphthyridinyl
	3*H*-Indole	3*H*-Indolyl		Quinoxaline	Quinoxalinyl
	Indole	Indolyl		Quinazoline	Quinazolinyl
	1*H*-Indazole	1*H*-Indazolyl		Cinnoline	Cinnolinyl
	Purine*	Purinyl		Pteridine	Pteridinyl
	4*H*-Quinolizine	4*H*-Quinolizinyl		4α*H*-Carbazole*	4α*H*-Carbazolyl
	Isoquinoline	Isoquinolyl			
	Quinolone	Quinolyl		Carbazole*	Carbazolyl

* Asterisk after a compound denotes exception to systematic numbering.

TABLE 1.5 Trivial Names of Heterocyclic Systems Suitable for Use in Fusion Names (*Continued*)

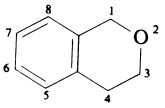
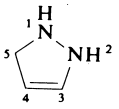
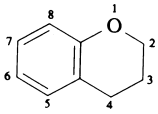
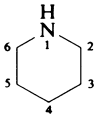
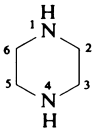
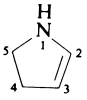
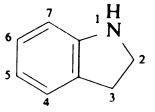
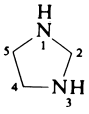
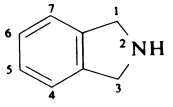
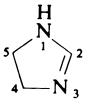
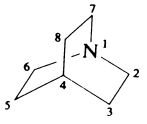
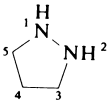
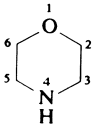
Structure	Parent name	Radical name	Structure	Parent name	Radical name
	β-Carboline	β-Carbolinyl		Phenazine	Phenazinyl
	Phenanthridine	Phenanthridinyl		Phenarsazine	Phenarsazinyl
	Acridine*	Acridinyl		Phenothiazine	Phenothiazinyl
	Perimidine	Perimidinyl		Furazan	Furazanyl
	Phenanthroline (1,10-shown)	Phenanthrolinyl		Phenoxazine	Phenoxazinyl

* Asterisk after a compound denotes exception to systematic numbering.

If there is a choice among heterocyclic systems, the parent compound is decided in the following order of preference:

1. A nitrogen-containing component
2. A component containing a heteroatom, in the absence of nitrogen, as high as possible in Table 1.3
3. A component containing the greater number of rings

TABLE 1.6 Trivial Names of Heterocyclic Systems That Are Not Recommended for Use in Fusion Names
Listed in order of increasing priority.

Structure	Parent name	Radical name	Structure	Parent name	Radical name
	Isochroman	Isochromanyl		Pyrazoline (3-shown*)	Pyrazolinyl
	Chroman	Chromanyl		Piperidine	Piperidyl†
	Pyrrolidine	Pyrrolinyl		Piperazine	Piperazinyl
	Pyrroline (2-shown*)	Pyrrolinyl		Indoline	Indolinyl
	Imidazolidine	Imidazolidinyl		Isoindoline	Isoindolinyl
	Imidazoline (2-shown*)	Imidazolinyl		Quinuclidine	Quinuclidinyl
	Pyrazolidine	Pyrazolidinyl		Morpholine	Morpholinyl‡

* Denotes position of double bond.
† For 1-piperidyl, use piperidino.
‡ For 4-morpholinyl, use morpholino.

4. A component containing the largest possible individual ring

5. A component containing the greatest number of heteroatoms of any kind

6. A component containing the greatest variety of heteroatoms

7. A component containing the greatest number of heteroatoms first listed in Table 1.3

If there is a choice between components of the same size containing the same number and kind of heteroatoms, choose as the base component that one with the lower numbers for the heteroatoms before fusion. When a fusion position is occupied by a heteroatom, the names of the component rings to be fused are selected to contain the heteroatom.

1.1.2 Functional Compounds

There are several types of nomenclature systems that are recognized. Which type to use is sometimes obvious from the nature of the compound. Substitutive nomenclature, in general, is preferred because of its broad applicability, but radicofunctional, additive, and replacement nomenclature systems are convenient in certain situations.

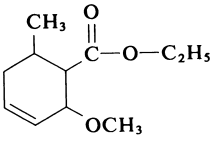
1.1.2.1 Substitutive Nomenclature. The first step is to determine the kind of characteristic (functional) group for use as the principal group of the parent compound. A characteristic group is a recognized combination of atoms that confers characteristic chemical properties on the molecule in which it occurs. Carbon-to-carbon unsaturation and heteroatoms in rings are considered nonfunctional for nomenclature purposes.

Substitution means the replacement of one or more hydrogen atoms in a given compound by some other kind of atom or group of atoms, functional or nonfunctional. In substitutive nomenclature, each substituent is cited as either a prefix or a suffix to the name of the parent (or substituting radical) to which it is attached; the latter is denoted the parent compound (or parent group if a radical).

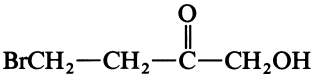
In Table 1.7 are listed the general classes of compounds in descending order of preference for citation as suffixes, that is, as the parent or characteristic compound. When oxygen is replaced by sulfur, selenium, or tellurium, the priority for these elements is in the descending order listed. The higher valence states of each element are listed before considering the successive lower valence states. Derivative groups have priority for citation as principal group after the respective parents of their general class.

In Table 1.8 are listed characteristic groups that are cited only as prefixes (never as suffixes) in substitutive nomenclature. The order of listing has no significance for nomenclature purposes.

Systematic names formed by applying the principles of substitutive nomenclature are single words except for compounds named as acids. First one selects the parent compound, and thus the suffix, from the characteristic group listed earliest in Table 1.7. All remaining functional groups are handled as prefixes that precede, in alphabetical order, the parent name. Two examples may be helpful:



Structure I



Structure II

Structure I contains an ester group and an ether group. Since the ester group has higher priority, the name is ethyl 2-methoxy-6-methyl-3-cyclohexene-1-carboxylate. Structure II contains a carbonyl group, a hydroxy group, and a bromo group. The latter is never a suffix. Between the other two, the carbonyl group has higher priority, the parent has -one as suffix, and the name is 4-bromo-1-hydroxy-2-butanone.

Selection of the principal alicyclic chain or ring system is governed by these selection rules:

1. For purely alicyclic compounds, the selection process proceeds successively until a decision is reached: (a) the maximum number of substituents corresponding to the characteristic group cited earliest in Table 1.7, (b) the maximum number of double and triple bonds considered together, (c) the maximum length of the chain, and (d) the maximum number of double bonds. Additional criteria, if needed for complicated compounds, are given in the IUPAC nomenclature rules.

2. If the characteristic group occurs only in a chain that carries a cyclic substituent, the compound is named as an aliphatic compound into which the cyclic component is substituted; a radical prefix is used to denote the cyclic component. This chain need not be the longest chain.

3. If the characteristic group occurs in more than one carbon chain and the chains are not directly

TABLE 1.7 Characteristic Groups for Substitutive Nomenclature

Listed in order of decreasing priority for citation as principal group or parent name.

Class	Formula*	Prefix	Suffix
1. Cations:		-onio-	-onium
	H_4N^+	Ammonio-	-ammonium
	H_3O^+	Oxonio-	-oxonium
	H_3S^+	Sulfonio-	-sulfonium
	H_3Se^+	Selenonio-	-selenonium
	H_2Cl^+	Chloronio-	-chloronium
	H_2Br^+	Bromonio-	-bromonium
	H_2I^+	Iodonio-	-iodonium
2. Acids:			
Carboxylic	—COOH	Carboxy-	-carboxylic acid
	—(C)OOH		-oic acid
	—C(=O)OOH		-peroxy···carboxylic acid
	—(C=O)OOH		-peroxy···oic acid
Sulfonic	$—SO_3H$	Sulfo-	-sulfonic acid
Sulfinic	$—SO_2H$	Sulfino-	-sulfinic acid
Sulfenic	—SOH	Sulfeno-	-sulfenic acid
Salts	—COOM		Metal···carboxylate
	—(C)OOM		Metal···oate
	$—SO_3M$		Metal···sulfonate
	$—SO_2M$		Metal···sulfinate
	—SOM		Metal···sulfenate
3. Derivatives of acids:			
Anhydrides	—C(=O)OC(=O)—		-carboxylic anhydride
	—(C=O)O(C=O)—		-oic anhydride
Esters	—COOR	R-oxycarbonyl-	R···carboxylate
	—C(OOR)		R···oate
Acid halides	—CO—halogen	Haloformyl	-carbonyl halide
Amides	$—CO—NH_2$	Carbamoyl-	-carboxamide
	$(C)O—NH_2$		-amide

TABLE 1.7 Characteristic Groups for Substitutive Nomenclature (*Continued*)

Class	Formula*	Prefix	Suffix
Hydrazides	—CO—$NHNH_2$	Carbonyl-hydrazino-	-carbohydrazide
	—(CO)—$NHNH_2$		-ohydrazide
Imides	—CO—NH—CO—	R-imido-	-carboximide
Amidines	—C(═NH)—NH_2	Amidino-	-carboxamidine
	—(C═NH)—NH_2		-amidine
4. Nitrile (cyanide)	—CN	Cyano-	-carbonitrile
	—(C)N		-nitrile
5. Aldehydes	—CHO	Formyl-	-carbaldehyde
	—(C═O)H	Oxo-	-al
	(then their analogs and derivatives)		
6. Ketones	＞(C═O)	Oxo-	-one
	(then their analogs and derivatives)		
7. Alcohols (and phenols)	—OH	Hydroxy-	-ol
Thiols	—SH	Mercapto-	-thiol
8. Hydroperoxides	—O—OH	Hydroperoxy-	
9. Amines	—NH_2	Amino-	-amine
Imines	＞NH	Imino-	-imine
Hydrazines	—$NHNH_2$	Hydrazino-	-hydrazine
10. Ethers	—OR	R-oxy-	
Sulfides	—SR	R-thio-	
11. Peroxides	—O—OR	R-dioxy-	

* Carbon atoms enclosed in parentheses are included in the name of the parent compound and not in the suffix or prefix.

TABLE 1.8 Characteristic Groups Cited Only as Prefixes in Substitutive Nomenclature

Characteristic group	Prefix	Characteristic group	Prefix
—Br	Bromo-	—IX_2	X may be halogen or a radical; dihalogenoiodo- or diacetoxyiodo-, e.g., —ICl_2 is dichloroido-
—Cl	Chloro-		
—ClO	Chlorosyl-		
—ClO_2	Chloryl-	＞N_2	Diazo-
—ClO_3	Perchloryl-	—N_3	Azido-
—F	Fluoro-	—NO	Nitroso-
—I	Iodo-	—NO_2	Nitro-
—IO	Iodosyl-	＞N(═O)OH	*aci*-Nitro-
—IO_2	Iodyl*	—OR	R-oxy-
—$I(OH)_2$	Dihydroxyiodo-	—SR	R-thio-
		—SeR (—TeR)	R-seleno- (R-telluro-)

* Formerly iodoxy.

attached to one another, then the chain chosen as parent should carry the largest number of the characteristic group. If necessary, the selection is continued as in rule 1.

4. If the characteristic group occurs only in one cyclic system, that system is chosen as the parent.
5. If the characteristic group occurs in more than one cyclic system, that system is chosen as parent which (a) carries the largest number of the principal group or, failing to reach a decision, (b) is the senior ring system.
6. If the characteristic group occurs both in a chain and in a cyclic system, the parent is that portion in which the principal group occurs in largest number. If the numbers are the same, that portion is chosen which is considered to be the most important or is the senior ring system.
7. When a substituent is itself substituted, all the subsidiary substituents are named as prefixes and the entire assembly is regarded as a parent radical.
8. The seniority of ring systems is ascertained by applying the following rules successively until a decision is reached: (a) all heterocycles are senior to all carbocycles, (b) for heterocycles, the preference follows the decision process described under Heterocyclic Systems, p. 1.11, (c) the largest number of rings, (d) the largest individual ring at the first point of difference, (e) the largest number of atoms in common among rings, (f) the lowest letters in the expression for ring functions, (g) the lowest numbers at the first point of difference in the expression for ring junctions, (h) the lowest state of hydrogenation, (i) the lowest-numbered locant for indicated hydrogen, (j) the lowest-numbered locant for point of attachment (if a radical), (k) the lowest-numbered locant for an attached group expressed as a suffix, (l) the maximum number of substituents cited as prefixes, (m) the lowest-numbered locant for substituents named as prefixes, hydro prefixes, -ene, and -yne, all considered together in one series in ascending numerical order independent of their nature, and (n) the lowest-numbered locant for the substituent named as prefix which is cited first in the name.

Numbering of Compounds. If the rules for aliphatic chains and ring systems leave a choice, the starting point and direction of numbering of a compound are chosen so as to give lowest-numbered locants to these structural factors, if present, considered successively in the order listed below until a decision is reached. Characteristic groups take precedence over multiple bonds.

1. Indicated hydrogen, whether cited in the name or omitted as being conventional
2. Characteristic groups named as suffix following the ranking order of Table 1.7
3. Multiple bonds in acyclic compounds; in bicycloalkanes, tricycloalkanes, and polycycloalkanes, double bonds having priority over triple bonds; and in heterocyclic systems whose names end in -etine, -oline, or -olene
4. The lowest-numbered locant for substituents named as prefixes, hydro prefixes, -ene, and -yne, all considered together in one series in ascending numerical order
5. The lowest locant for that substituent named as prefix which is cited first in the name

For cyclic radicals, indicated hydrogen and thereafter the point of attachment (free valency) have priority for the lowest available number.

Prefixes and Affixes. Prefixes are arranged alphabetically and placed before the parent name; multiplying affixes, if necessary, are inserted and *do not* alter the alphabetical order already attained. The parent name includes any syllables denoting a change of ring member or relating to the structure of a carbon chain. Nondetachable parts of parent names include

1. Forming rings; cyclo-, bicyclo-, spiro-

2. Fusing two or more rings: benzo-, naphtho-, imidazo-

3. Substituting one ring or chain member atom for another: oxa-, aza-, thia-

4. Changing positions of ring or chain members: iso-, *sec*-, *tert*-, neo-

5. Showing indicated hydrogen

6. Forming bridges: ethano-, epoxy-

7. Hydro-

Prefixes that represent complete terminal characteristic groups are preferred to those representing only a portion of a given group. For example, for the prefix —C(═O)CH_3, the name (formylmethyl) is preferred to (oxoethyl).

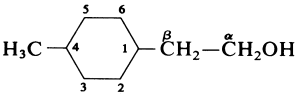
The multiplying affixes di-, tri-, tetra-, penta-, hexa-, hepta-, octa-, nona-, deca-, undeca-, and so on are used to indicate a set of *identical* unsubstituted radicals or parent compounds. The forms bis-, tris-, tetrakis-, pentakis-, and so on are used to indicate a set of identical radicals or parent compounds *each substituted in the same way.* The affixes bi-, ter-, quater-, quinque-, sexi-, septi-, octi-, novi-, deci-, and so on are used to indicate the number of identical rings joined together by a single or double bond.

Although multiplying affixes may be omitted for very common compounds when no ambiguity is caused thereby, such affixes are generally included throughout this handbook in alphabetical listings. An example would be ethyl ether for diethyl ether.

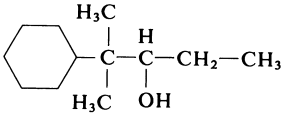
1.1.2.2 Conjunctive Nomenclature. Conjunctive nomenclature may be applied when a principal group is attached to an acyclic component that is directly attached by a carbon-carbon bond to a cyclic component. The name of the cyclic component is attached directly in front of the name of the acyclic component carrying the principal group. This nomenclature is not used when an unsaturated side chain is named systematically. When necessary, the position of the side chain is indicated by a locant placed before the name of the cyclic component. For substituents on the acyclic chain, carbon atoms of the side chain are indicated by Greek letters proceeding from the principal group to the cyclic component. The terminal carbon atom of acids, aldehydes, and nitriles is omitted when allocating Greek positional letters. Conjunctive nomenclature is not used when the side chain carries more than one of the principal group, except in the case of malonic and succinic acids.

The side chain is considered to extend only from the principal group to the cyclic component. Any other chain members are named as substituents, with appropriate prefixes placed before the name of the cyclic component.

When a cyclic component carries more than one identical side chain, the name of the cyclic component is followed by di-, tri-, etc., and then by the name of the acyclic component, and it is preceded by the locants for the side chains. Examples are



4-Methyl-1-cyclohexaneethanol



α-Ethyl-β,β-dimethylcyclohexaneethanol

When side chains of two or more different kinds are attached to a cyclic component, only the senior side chain is named by the conjunctive method. The remaining side chains are named as prefixes. Likewise, when there is a choice of cyclic component, the senior is chosen. Benzene derivatives may be named by the conjunctive method only when two or more identical side chains are present. Trivial names for oxo carboxylic acids may be used for the acyclic component. If the cyclic and acyclic components are joined by a double bond, the locants of this bond are placed as superscripts to a Greek capital delta that is inserted between the two names. The locant for the cyclic component precedes that for the acyclic component, e.g., indene-$\Delta^{1,\alpha}$-acetic acid.

1.1.2.3 Radicofunctional Nomenclature. The procedures of radicofunctional nomenclature are identical with those of substitutive nomenclature except that suffixes are never used. Instead, the functional class name (Table 1.9) of the compound is expressed as one word and the remainder of the molecule as another that precedes the class name. When the functional class name refers to a characteristic group that is bivalent, the two radicals attached to it are each named, and when different, they are written as separate words arranged in alphabetical order. When a compound contains more than one kind of group listed in Table 1.9, that kind is cited as the functional group or class name that occurs higher in the table, all others being expressed as prefixes.

Radicofunctional nomenclature finds some use in naming ethers, sulfides, sulfoxides, sulfones, selenium analogs of the preceding three sulfur compounds, and azides.

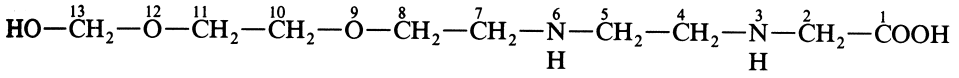
TABLE 1.9 Functional Class Names Used in Radicofunctional Nomenclature

Groups are listed in order of decreasing priority.

Group	Functional class names
X in acid derivatives	Name of X (in priority order: fluoride, chloride, bromide, iodide, cyanide, azide; then the sulfur and selenium analogs)
—CN, —NC	Cyanide, isocyanide
>CO	Ketone; then S and Se analogs
—OH	Alcohol; then S and Se analogs
—O—OH	Hydroperoxide
>O	Ether or oxide
>S, >SO, $>SO_2$	Sulfide, sulfoxide, sulfone
>Se, >SeO, $>SeO_2$	Selenide, selenoxide, selenone
—F, —Cl, —Br, —I	Fluoride, chloride, bromide, iodide
$—N_3$	Azide

1.1.2.4 Replacement Nomenclature. Replacement nomenclature is intended for use only when other nomenclature systems are difficult to apply in the naming of chains containing heteroatoms. When no group is present that can be named as a principal group, the longest chain of carbon and heteroatoms terminating with carbon is chosen and named as though the entire chain were that of an acyclic hydrocarbon. The heteroatoms within this chain are identified by means of prefixes aza-, oxa-, thia-, etc., in the order of priority stated in Table 1.3. Locants indicate the positions of the heteroatoms in the chain. Lowest-numbered locants are assigned to the principal group when

such is present. Otherwise, lowest-numbered locants are assigned to the heteroatoms considered together and, if there is a choice, to the heteroatoms cited earliest in Table 1.3. An example is



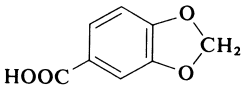
13-Hydroxy-9,12-dioxa-3,6-diazatridecanoic acid

1.1.3 Specific Functional Groups

Characteristic groups will now be treated briefly in order to expand the terse outline of substitutive nomenclature presented in Table 1.7. Alternative nomenclature will be indicated whenever desirable.

1.1.3.1 Acetals and Acylals. Acetals, which contain the group $>C(OR)_2$, where R may be different, are named (1) as dialkoxy compounds or (2) by the name of the corresponding aldehyde or ketone followed by the name of the hydrocarbon radical(s) followed by the word *acetal*. For example, $CH_3—CH(OCH_3)_2$ is named either (1) 1,1-dimethoxyethane or (2) acetaldehyde dimethyl acetal.

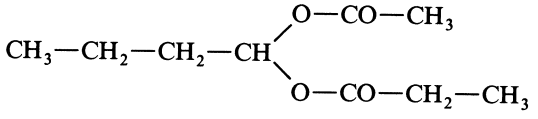
A cyclic acetal in which the two acetal oxygen atoms form part of a ring may be named (1) as a heterocyclic compound or (2) by use of the prefix methylenedioxy for the group $—O—CH_2—O—$ as a substituent in the remainder of the molecule. For example,



(1) 1,3-Benzo[*d*]dioxole-5-carboxylic acid

(2) 3,4-Methylenedioxybenzoic acid

Acylals, $R^1R^2C(OCOR^3)_2$, are named as acid esters;



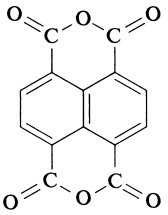
Butylidene acetate propionate

α-Hydroxy ketones, formerly called acyloins, had been named by changing the ending -ic acid or -oic acid of the corresponding acid to -oin. They are preferably named by substitutive nomenclature; thus

$CH_3—CH(OH)—CO—CH_3$ 3-Hydroxy-2-butanone (formerly acetoin)

1.1.3.2 Acid Anhydrides. Symmetrical anhydrides of monocarboxylic acids, when unsubstituted, are named by replacing the word *acid* by *anhydride*. Anhydrides of substituted monocarboxylic acids, if symmetrically substituted, are named by prefixing bis- to the name of the acid and replacing the word *acid* by *anhydride*. Mixed anhydrides are named by giving in alphabetical order the first part of the names of the two acids followed by the word *anhydride*, e.g., acetic propionic anhydride or acetic propanoic anhydride. Cyclic anhydrides of polycarboxylic acids, although possessing a

heterocyclic structure, are preferably named as acid anhydrides. For example,



1,8;4,5-Napthalenetetracarboxylic dianhydride (note the use of a semicolon to distinguish the pairs of locants)

1.1.3.3 Acyl Halides. Acyl halides, in which the hydroxyl portion of a carboxyl group is replaced by a halogen, are named by placing the name of the corresponding halide after that of the acyl radical. When another group is present that has priority for citation as principal group or when the acyl halide is attached to a side chain, the prefix haloformyl- is used as, for example, in fluoroformyl-.

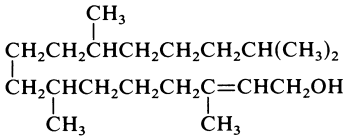
1.1.3.4 Alcohols and Phenols. The hydroxyl group is indicated by a suffix -ol when it is the principal group attached to the parent compound and by the prefix hydroxy- when another group with higher priority for citation is present or when the hydroxy group is present in a side chain. When confusion may arise in employing the suffix -ol, the hydroxy group is indicated as a prefix; this terminology is also used when the hydroxyl group is attached to a heterocycle, as, for example, in the name 3-hydroxythiophene to avoid confusion with thiophenol (C_6H_5SH). Designations such as isopropanol, *sec*-butanol, and *tert*-butanol are incorrect because no hydrocarbon exists to which the suffix can be added. Many trivial names are retained. These structures are shown in Table 1.10. The radicals (RO—) are named by adding -oxy as a suffix to the name of the R radical, e.g., pentyloxy for $CH_3CH_2CH_2CH_2CH_2O$—. These contractions are exceptions: methoxy (CH_3O—), ethoxy (C_2H_5O—), propoxy (C_3H_7O—), butoxy (C_4H_9O—), and phenoxy (C_6H_5O—). For unsubstituted radicals only, one may use isopropoxy [$(CH_3)_2CH$—O—], isobutoxy [$(CH_3)_2CH_2CH$—O—], *sec*-butoxy [$CH_3CH_2CH(CH_3)$—O—], and *tert*-butoxy [$(CH_3)_3C$—O—].

TABLE 1.10 Retained Trivial Names of Alcohols and Phenols with Structures

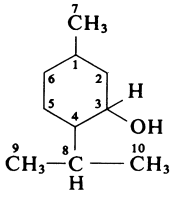
Ally alcohol	$CH_2{=}CHCH_2OH$
tert-Butyl alcohol	$(CH_3)_3COH$
Benzyl alcohol	$C_6H_5CH_2OH$
Phenethyl alcohol	$C_6H_5CH_2CH_2OH$
Ethylene glycol	$HOCH_2CH_2OH$
1,2-Propylene glycol	$CH_3CHOHCH_2OH$
Glycerol	$HOCH_2CHOHCH_2OH$
Pentaerythritol	$C(CH_2OH)_4$
Pinacol	$(CH_3)_2COHCOH(CH_3)_2$
Phenol	C_6H_5OH
Xylitol	$HOCH_2CH(OH)—CH(OH)—CH(OH)—CH_2OH$
Geraniol	$(CH_3)_2C{=}CHCH_2CH_2C(CH_3){=}CHCH_2OH$

TABLE 1.10 Retained Trivial Names of Alcohols and Phenols with Structures (*Continued*)

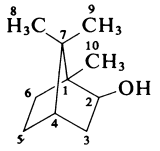
Phytol

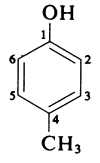


Menthol

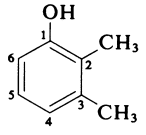


Borneol

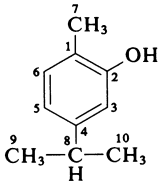




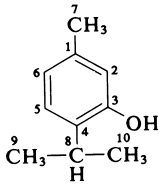
Cresol (1,4-isomer shown)



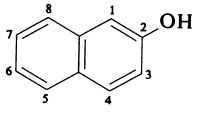
Xylenol (2,3-isomer shown)



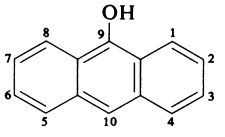
Carvacrol



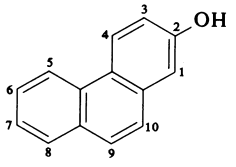
Thymol



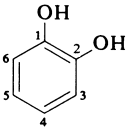
Naphthol (2-isomer shown)
2-Hydroxynaphthalene



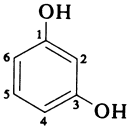
Anthrol (9-isomer shown)
9-Hydroxyanthracene



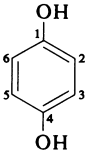
Phenanthrol (2-isomer shown)
2-Hydroxyphenanthrene



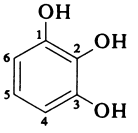
Pyrocatechol
1,2-Dihydroxybenzene



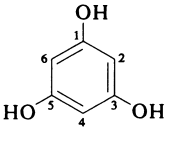
Resorcinol
1,3-Dihydroxybenzene



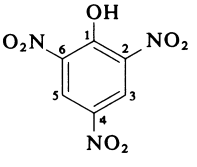
Hydroquinone
1,4-Dihydroxybenzene



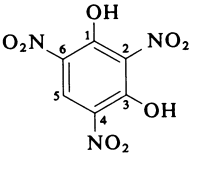
Pyrogallol
1,2,3-Trihydroxybenzene



Phloroglucinol
1,3,5-Trihydroxybenzene



Picric acid
2,4,6-Trinitrophenol



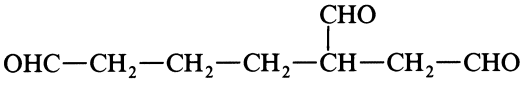
Styphnic acid
1,3-Dihydroxy-2,4,6-trinitroben-
zene

Bivalent radicals of the form O—Y—O are named by adding -dioxy to the name of the bivalent radicals except when forming part of a ring system. Examples are —O—CH_2—O— (methylenedioxy), —O—CO—O— (carbonyldioxy), and —O—SO_2—O— (sulfonyldioxy). Anions derived from alcohols or phenols are named by changing the final -ol to -olate.

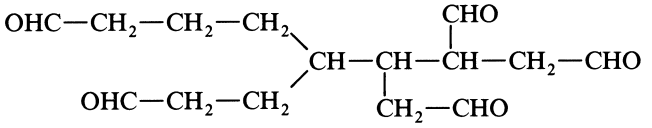
Salts composed of an anion, RO—, and a cation, usually a metal, can be named by citing first the cation and then the RO anion (with its ending changed to -yl oxide), e.g., sodium benzyl oxide for $C_6H_5CH_2ONa$. However, when the radical has an abbreviated name, such as methoxy, the ending -oxy is changed to -oxide. For example, CH_3ONa is named sodium methoxide (not sodium methylate).

1.1.3.5 Aldehydes. When the group —C(=O)H, usually written —CHO, is attached to carbon at one (or both) end(s) of a linear acyclic chain the name is formed by adding the suffix -al (or -dial) to the name of the hydrocarbon containing the same number of carbon atoms. Examples are butanal for $CH_3CH_2CH_2CHO$ and propanedial for, $OHCCH_2CHO$.

Naming an acyclic polyaldehyde can be handled in two ways. First, when more than two aldehyde groups are attached to an unbranched chain, the proper affix is added to -carbaldehyde, which becomes the suffix to the name of the longest chain carrying the maximum number of aldehyde groups. The name and numbering of the main chain do not include the carbon atoms of the aldehyde groups. Second, the name is formed by adding the prefix formyl- to the name of the -dial that incorporates the principal chain. Any other chains carrying aldehyde groups are named by the use of formylalkyl- prefixes. Examples are



(1) 1,2,5-Pentanetricarbaldehyde
(2) 3-Formylheptanedial



(1) 4-(2-Formylethyl)-3-(formylmethyl)-1,2,7-heptanetricarbaldehyde
(2) 3-Formyl-5-(2-formylethyl)-4-(formylmethyl)nonanedial

When the aldehyde group is directly attached to a carbon atom of a ring system, the suffix -carbaldehyde is added to the name of the ring system, e.g., 2-naphthalenecarbaldehyde. When the aldehyde group is separated from the ring by a chain of carbon atoms, the compound is named (1) as a derivative of the acyclic system or (2) by conjunctive nomenclature, for example, (1) (2-naphthyl)propionaldehyde or (2) 2-naphthalenepropionaldehyde.

An aldehyde group is denoted by the prefix formyl- when it is attached to a nitrogen atom in a ring system or when a group having priority for citation as principal group is present and part of a cyclic system.

When the corresponding monobasic acid has a trivial name, the name of the aldehyde may be formed by changing the ending -ic acid or -oic acid to -aldehyde. Examples are

Formaldehyde	Acrylaldehyde (not acrolein)
Acetaldehyde	Benzaldehyde
Propionaldehyde	Cinnamaldehyde
Butyraldehyde	2-Furaldehyde (not furfural)

The same is true for polybasic acids, with the proviso that all the carboxyl groups must be changed to aldehyde; then it is not necessary to introduce affixes. Examples are

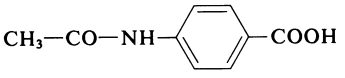
Glyceraldehyde	Succinaldehyde
Glycolaldehyde	Phthalaldehyde (*o*-, *m*-, *p*-)
Malonaldehyde	

These trivial names may be retained: citral (3,7-dimethyl-2,6-octadienal), vanillin (4-hydroxy-3-methoxybenzaldehyde), and piperonal (3,4-methylenedioxybenzaldehyde).

1.1.3.6 Amides. For primary amides the suffix -amide is added to the systematic name of the parent acid. For example, $CH_3—CO—NH_2$ is acetamide. Oxamide is retained for $H_2N—CO—CO—NH_2$. The name -carboxylic acid is replaced by -carboxamide.

For amino acids having trivial names ending in -ine, the suffix -amide is added after the name of the acid (with elision of *e* for monoamides). For example, $H_2N—CH_2—CO—NH_2$ is glycinamide.

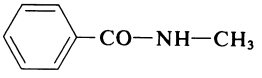
In naming the radical R—CO—NH—, either (1) the -yl ending of RCO— is changed to -amido or (2) the radicals are named as acylamino radicals. For example,



(1) 4-Acetamidobenzoic acid
(2) 4-Acetylaminobenzoic acid

The latter nomenclature is always used for amino acids with trivial names.

N-substituted primary amides are named either (1) by citing the substituents as *N* prefixes or (2) by naming the acyl group as an *N* substituent of the parent compound. For example,



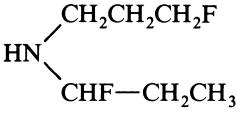
(1) *N*-Methylbenzamide
(2) Benzoylaminomethane

1.1.3.7 Amines. Amines are preferably named by adding the suffix -amine (and any multiplying affix) to the name of the parent radical. Examples are

$CH_3CH_2CH_2CH_2CH_2NH_2$ Pentylamine

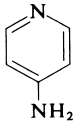
$H_2NCH_2CH_2CH_2CH_2CH_2NH_2$ 1,5-Pentyldiamine or pentamethylenediamine

Locants of substituents of symmetrically substituted derivatives of symmetrical amines are distinguished by primes or else the names of the complete substituted radicals are enclosed in parentheses. Unsymmetrically substituted derivatives are named similarly or as *N*-substituted products of a primary amine (after choosing the most senior of the radicals to be the parent amine). For example,



(1) 1,3′-Difluorodipropylamine
(2) 1-Fluoro-*N*-(3-fluoropropyl)propylamine
(3) (1-Fluoropropyl)(3-fluoropropyl)amine

Complex cyclic compounds may be named by adding the suffix -amine or the prefix amino- (or aminoalkyl-) to the name of the parent compound. Thus three names are permissible for



(1) 4-Pyridylamine
(2) 4-Pyridinamine
(3) 4-Aminopyridine

Complex linear polyamines are best designated by replacement nomenclature. These trivial names are retained: aniline, benzidene, phenetidine, toluidine, and xylidine.

The bivalent radical —NH— linked to two identical radicals can be denoted by the prefix imino-, as well as when it forms a bridge between two carbon ring atoms. A trivalent nitrogen atom linked to three identical radicals is denoted by the prefix nitrilo-. Thus ethylenediaminetetraacetic acid (an allowed exception) should be named ethylenedinitrilotetraacetic acid.

1.1.3.8 Ammonium Compounds. Salts and hydroxides containing quadricovalent nitrogen are named as a substituted ammonium salt or hydroxide. The names of the substituting radicals precede the word *ammonium*, and then the name of the anion is added as a separate word. For example, $(CH_3)_4N^+I^-$ is tetramethylammonium iodide.

When the compound can be considered as derived from a base whose name does not end in -amine, its quaternary nature is denoted by adding ium to the name of that base (with elision of *e*), substituent groups are cited as prefixes, and the name of the anion is added separately at the end. Examples are

$C_6H_5NH_3^+HSO_4^-$ Anilinium hydrogen sulfate

$[(C_6H_5NH_3)^+]_2PtCl_6^{2-}$ Dianilinium hexachloroplatinate

The names *choline* and *betaine* are retained for unsubstituted compounds.

In complex cases, the prefixes amino- and imino- may be changed to ammonio- and iminio- and are followed by the name of the molecule representing the most complex group attached to this nitrogen atom and are preceded by the names of the other radicals attached to this nitrogen. Finally the name of the anion is added separately. For example, the name might be 1-trimethylammonioacridine chloride or 1-acridinyltrimethylammonium chloride.

When the preceding rules lead to inconvenient names, then (1) the unaltered name of the base may be used followed by the name of the anion or (2) for salts of hydrohalogen acids only the unaltered name of the base is used followed by the name of the hydrohalide. An example of the latter would be 2-ethyl-*p*-phenylenediamine monohydrochloride.

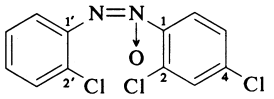
1.1.3.9 Azo Compounds. When the azo group (—N═N—) connects radicals derived from identical unsubstituted molecules, the name is formed by adding the prefix azo- to the name of the parent unsubstituted molecules. Substituents are denoted by prefixes and suffixes. The azo group has priority for lowest-numbered locant. Examples are azobenzene for $C_6H_5—N═N—C_6H_5$, azobenzene-4-sulfonic acid for $C_6H_5—N═N—C_6H_5SO_3H$, and 2′,4-dichloroazobenzene-4′-sulfonic acid for $ClC_6H_4—N═N—C_6H_3ClSO_3H$.

When the parent molecules connected by the azo group are different, azo is placed between the complete names of the parent molecules, substituted or unsubstituted. Locants are placed between the affix azo and the names of the molecules to which each refers. Preference is given to the more complex parent molecule for citation as the first component, e.g., 2-aminonaphthalene-1-azo-(4′-chloro-2′-methylbenzene).

In an alternative method, the senior component is regarded as substituted by RN═N—, this group R being named as a radical. Thus 2-(7-phenylazo-2-naphthylazo)anthracene is the name by this alternative method for the compound named anthracene-2-azo-2′-naphthalene-7′-azobenzene.

1.1.3.10 Azoxy Compounds. Where the position of the azoxy oxygen atom is unknown or immaterial, the compound is named in accordance with azo rules, with the affix azo replaced by azoxy. When the position of the azoxy oxygen atom in an unsymmetrical compound is designated, a prefix *NNO*- or *ONN*- is used. When both the groups attached to the azoxy radical are cited in the name of the compound, the prefix *NNO*- specifies that the second of these two groups is attached directly

to —N(O)—; the prefix *ONN*- specifies that the first of these two groups is attached directly to —N(O)—. When only one parent compound is cited in the name, the prefixed *ONN*- and *NNO*- specify that the group carrying the primed and unprimed substituents is connected, respectively, to the —N(O)— group. The prefix *NON*- signifies that the position of the oxygen atom is unknown; the azoxy group is then written as $—N_2O—$. For example,



2,2′,4-Trichloro-*NNO*-azoxybenzene

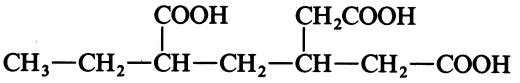
1.1.3.11 Boron Compounds. Molecular hydrides of boron are called boranes. They are named by using a multiplying affix to designate the number of boron atoms and adding an Arabic numeral within parentheses as a suffix to denote the number of hydrogen atoms present. Examples are pentaborane(9) for B_5H_9 and pentaborane(11) for B_5H_{11}.

Organic ring systems are named by replacement nomenclature. Three- to ten-membered monocyclic ring systems containing uncharged boron atoms may be named by the specialist nomenclature for heterocyclic systems. Organic derivatives are named as outlined for substitutive nomenclature. The complexity of boron nomenclature precludes additional details; the text by Rigaudy and Klesney should be consulted.

1.1.3.12 Carboxylic Acids. Carboxylic acids may be named in several ways. First, —COOH groups replacing CH_3— at the end of the main chain of an acyclic hydrocarbon are denoted by adding -oic acid to the name of the hydrocarbon. Second, when the —COOH group is the principal group, the suffix -carboxylic acid can be added to the name of the parent chain whose name and chain numbering *does not include* the carbon atom of the —COOH group. The former nomenclature is preferred unless use of the ending -carboxylic acid leads to citation of a larger number of carboxyl groups as suffix. Third, carboxyl groups are designated by the prefix carboxy- when attached to a group named as a substituent or when another group is present that has higher priority for citation as principal group. In all cases, the principal chain should be linked to as many carboxyl groups as possible even though it might not be the longest chain present. Examples are

$CH_3CH_2CH_2CH_2CH_2CH_2COOH$ (1) Heptanoic acid
(2) 1-Hexanecarboxylic acid

$C_6H_{11}COOH$ (2) Cyclohexanecarboxylic acid



(3) 2-(Carboxymethyl)-1,4-hexanedicarboxylic acid

Removal of the OH from the —COOH group to form the acyl radical results in changing the ending -oic acid to -oyl or the ending -carboxylic acid to -carbonyl. Thus the radical $CH_3CH_2CH_2CH_2CO$— is named either pentanoyl or butanecarbonyl. When the hydroxyl has not been removed from all carboxyl groups present in an acid, the remaining carboxyl groups are denoted by the prefix carboxy-. For example, $HOOCCH_2CH_2CH_2CH_2CO$— is named 6-carboxyhexanoyl.

TABLE 1.11 Names of Some Carboxylic Acids

Systematic name	Trivial name	Systematic name	Trivial name
Methanoic	Formic	*trans*-Methylbutenedioic	Mesaconic*
Ethanoic	Acetic		
Propanoic	Propionic	1,2,2-Trimethyl-1,3-cyclopentanedicarboxylic acid	Camphoric
Butanoic	Butyric		
2-Methylpropanoic	Isobutyric*		
Pentanoic	Valeric	Benzenecarboxylic	Benzoic
3-Methylbutanoic	Isovaleric*	1,2-Benzenedicarboxylic	Phthalic
2,2-Dimethylpropanoic	Pivalic*	1,3-Benzenedicarboxylic	Isophthalic
Hexanoic	(Caproic)	1,4-Benzenedicarboxylic	Terephthalic
Heptanoic	(Enanthic)	Naphthalenecarboxylic	Naphthoic
Octanoic	(Caprylic)	Methylbenzenecarboxylic	Toluic
Decanoic	(Capric)	2-Phenylpropanoic	Hydratropic
Dodecanoic	Lauric*	2-Phenylpropenoic	Atropic
Tetradecanoic	Myristic*	*trans*-3-Phenylpropenoic	Cinnamic
Hexadecanoic	Palmitic*	Furancarboxylic	Furoic
Octadecanoic	Stearic*	Thiophenecarboxylic	Thenoic
		3-Pyridinecarboxylic	Nicotinic
Ethanedioic	Oxalic	4-Pyridinecarboxylic	Isonicotinic
Propanedioic	Malonic		
Butanedioic	Succinic	Hydroxyethanoic	Glycolic
Pentanedioic	Glutaric	2-Hydroxypropanoic	Lactic
Hexanedioic	Adipic	2,3-Dihydroxypropanoic	Glyceric
Heptanedioic	Pimelic*	Hydroxypropanedioic	Tartronic
Octanedioic	Suberic*	Hydroxybutanedioic	Malic
Nonanedioic	Azelaic*	2,3-Dihydroxybutanedioic	Tartaric
Decanedioic	Sebacic*	3-Hydroxy-2-phenylpropanoic	Tropic
Propenoic	Acrylic	2-Hydroxy-2,2-diphenylethanoic	Benzilic
Propynoic	Propiolic		
2-Methylpropenoic	Methacrylic	2-Hydroxybenzoic	Salicylic
trans-2-Butenoic	Crotonic	Methoxybenzoic	Anisic
cis-2-Butenoic	Isocrotonic	4-Hydroxy-3-methoxybenzoic	Vanillic
cis-9-Octadecenoic	Oleic		
trans-9-Octadecenoic	Elaidic	3,4-Dimethoxybenzoic	Veratric
cis-Butenedioic	Maleic	3,4-Methylenedioxybenzoic	Piperonylic
trans-Butenedioic	Fumaric	3,4-Dihydroxybenzoic	Protocatechuic
cis-Methylbutenedioic	Citraconic*	3,4,5-Trihydroxybenzoic	Gallic

* Systematic names should be used in derivatives formed by substitution on a carbon atom.
Note: The names in parentheses are abandoned but are listed for reference to older literature.

Many trivial names exist for acids; these are listed in Table 1.11. Generally, radicals are formed by replacing -ic acid by -oyl.* When a trivial name is given to an acyclic monoacid or diacid, the numeral 1 is always given as locant to the carbon atom of a carboxyl group in the acid or to the carbon atom with a free valence in the radical RCO—.

* Exceptions: formyl, acetyl, propionyl, butyryl, isobutyryl, valeryl, isovaleryl, oxalyl, malonyl, succinyl, glutaryl, furoyl, and thenoyl.

1.1.3.13 Ethers ($R^1—O—R^2$). In substitutive nomenclature, one of the possible radicals, R—O—, is stated as the prefix to the parent compound that is senior from among R^1 or R^2. Examples are methoxyethane for $CH_3OCH_2CH_3$ and butoxyethanol for $C_4H_9OCH_2CH_2OH$.

When another principal group has precedence and oxygen is linking two identical parent compounds, the prefix oxy- may be used, as with 2,2′-oxydiethanol for $HOCH_2CH_2OCH_2CH_2OH$.

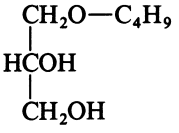
Compounds of the type RO—Y—OR, where the two parent compounds are identical and contain a group having priority over ethers for citation as suffix, are named as assemblies of identical units. For example, $HOOC—CH_2—O—CH_2CH_2—O—CH_2—COOH$ is named 2,2′-(ethylenedioxy)diacetic acid.

Linear polyethers derived from three or more molecules of aliphatic dihydroxy compounds, particularly when the chain length exceeds ten units, are most conveniently named by open-chain replacement nomenclature. For example, $CH_3CH_2—O—CH_2CH_2—O—CH_2CH_3$ could be 3,6-dioxaoctane or (2-ethoxy)ethoxyethane.

An oxygen atom directly attached to two carbon atoms already forming part of a ring system or to two carbon atoms of a chain may be indicated by the prefix epoxy-. For example, $CH_2—CH—CH_2Cl$ is named 1-chloro-2,3-epoxypropane.

Symmetrical linear polyethers may be named (1) in terms of the central oxygen atom when there is an odd number of ether oxygen atoms or (2) in terms of the central hydrocarbon group when there is an even number of ether oxygen atoms. For example, $C_2H_5—O—C_4H_8—O—C_4H_8—O—C_2H_5$ is bis-(4-ethoxybutyl)ether, and 3,6-dioxaoctane (earlier example) could be named 1,2-bis(ethoxy)ethane.

Partial ethers of polyhydroxy compounds may be named (1) by substitutive nomenclature or (2) by stating the name of the polyhydroxy compound followed by the name of the etherifying radical(s) followed by the word *ether*. For example,



(1) 3-Butoxy-1,2-propanediol
(2) Glycerol 1-butyl ether; also, 1-*O*-butylglycerol

Cyclic ethers are named either as heterocyclic compounds or by specialist rules of heterocyclic nomenclature. Radicofunctional names are formed by citing the names of the radicals R^1 and R^2 followed by the word *ether*. Thus methoxyethane becomes ethyl methyl ether and ethoxyethane becomes diethyl ether.

1.1.3.14 Halogen Derivatives. Using substitutive nomenclature, names are formed by adding prefixes listed in Table 1.8 to the name of the parent compound. The prefix perhalo- implies the replacement of all hydrogen atoms by the particular halogen atoms.

Cations of the type $R^1R^2X^+$ are given names derived from the halonium ion, H_2X^+, by substitution, e.g., diethyliodonium chloride for $(C_2H_5)_2I^+Cl^-$.

Retained are these trivial names; bromoform ($CHBr_3$), chloroform ($CHCl_3$), fluoroform (CHF_3), iodoform (CHI_3), phosgene ($COCl_2$), thiophosgene ($CSCl_2$), and dichlorocarbene radical ($\rangle CCl_2$). Inorganic nomenclature leads to such names as carbonyl and thiocarbonyl halides (COX_2 and CSX_2) and carbon tetrahalides (CX_4).

1.1.3.15 Hydroxylamines and Oximes. For RNH—OH compounds, prefix the name of the radical R to hydroxylamine. If another substituent has priority as principal group, attach the prefix

hydroxyamino- to the parent name. For example, C_6H_5NHOH would be named *N*-phenylhydroxylamine, but HOC_6H_4NHOH would be (hydroxyamino)phenol, with the point of attachment indicated by a locant preceding the parentheses.

Compounds of the type $R^1NH—OR^2$ are named (1) as alkoxyamino derivatives of compound R^1H, (2) as *N*,*O*-substituted hydroxylamines, (3) as alkoxyamines (even if R^1 is hydrogen), or (4) by the prefix aminooxy- when another substituent has priority for parent name. Examples of each type are

1. 2-(Methoxyamino)-8-naphthalenecarboxylic acid for $CH_3ONH—C_{10}H_6COOH$

2. *O*-Phenylhydroxylamine for $H_2N—O—C_6H_5$ or *N*-phenylhydroxylamine for $C_6H_5NH—OH$

3. Phenoxyamine for $H_2N—O—C_6H_5$ (not preferred to *O*-phenylhydroxylamine)

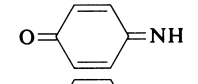
4. Ethyl (aminooxy)acetate for $H_2N—O—CH_2CO—OC_2H_5$

Acyl derivatives, $RCO—NH—OH$ and $H_2N—O—CO—R$, are named as *N*-hydroxy derivatives of amides and as *O*-acylhydroxylamines, respectively. The former may also be named as hydroxamic acids. Examples are *N*-hydroxyacetamide for $CH_3CO—NH—OH$ and *O*-acetylhydroxylamine for $H_2N—O—CO—CH_3$. Further substituents are denoted by prefixes with *O*- and/or *N*-locants. For example, $C_6H_5NH—O—C_2H_5$ would be *O*-ethyl-*N*-phenylhydroxylamine or *N*-ethoxylaniline.

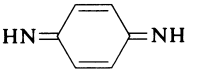
For oximes, the word *oxime* is placed after the name of the aldehyde or ketone. If the carbonyl group is not the principal group, use the prefix hydroxyimino-. Compounds with the group $\geq N—OR$ are named by a prefix alkyloxyimino- as oxime *O*-ethers or as *O*-substituted oximes. Compounds with the group $\geq C{=}N(O)R$ are named by adding *N*-oxide after the name of the alkylideneaminc compound. For amine oxides, add the word *oxide* after the name of the base, with locants. For example, $C_5H_5N—O$ is named pyridine *N*-oxide or pyridine 1-oxide.

1.1.3.16 Imines. The group $>C{=}NH$ is named either by the suffix -imine or by citing the name of the bivalent radical $R^1R^2C<$ as a prefix to amine. For example, $CH_3CH_2CH_2CH{=}NH$ could be named 1-butanimine or butylideneamine. When the nitrogen is substituted, as in $CH_2{=}N—CH_2CH_3$, the name is *N*-(methylidene)ethylamine.

Quinones are exceptions. When one or more atoms of quinonoid oxygen have been replaced by $>NH$ or $>NR$, they are named by using the name of the quinone followed by the word *imine* (and preceded by proper affixes). Substituents on the nitrogen atom are named as prefixes. Examples are



p-Benzoquinone monoimine

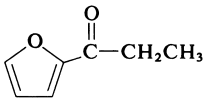


p-Benzoquinone diimine

1.1.3.17 Ketenes. Derivatives of the compound ketene, $CH_2{=}C{=}O$, are named by substitutive nomenclature. For example, $C_4H_9CH{=}C{=}O$ is butyl ketene. An acyl derivative, such as $CH_3CH_2—CO—CH_2CH{=}C{=}O$, may be named as a polyketone, 1-hexene-1,4-dione. Bisketene is used for two to avoid ambiguity with diketene (dimeric ketene).

1.1.3.18 Ketones. Acyclic ketones are named (1) by adding the suffix -one to the name of the hydrocarbon forming the principal chain or (2) by citing the names of the radicals R^1 and R^2 followed

by the word *ketone.* In addition to the preceding nomenclature, acyclic monoacyl derivatives of cyclic compounds may be named (3) by prefixing the name of the acyl group to the name of the cyclic compound. For example, the three possible names of

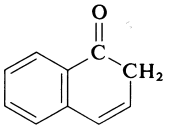


(1) 1-(2-Furyl)-1-propanone
(2) Ethyl 2-furyl ketone
(3) 2-Propionylfuran

When the cyclic component is benzene or naphthalene, the -ic acid or -oic acid of the acid corresponding to the acyl group is changed to -ophenone or -onaphthone, respectively. For example, $C_6H_5—CO—CH_2CH_2CH_3$ can be named either butyrophenone (or butanophenone) or phenyl propyl ketone.

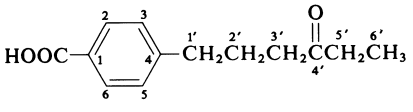
Radicofunctional nomenclature can be used when a carbonyl group is attached directly to carbon atoms in two ring systems and no other substituent is present having priority for citation.

When the methylene group in polycarbocyclic and heterocyclic ketones is replaced by a keto group, the change may be denoted by attaching the suffix -one to the name of the ring system. However, when $\geq CH$ in an unsaturated or aromatic system is replaced by a keto group, two alternative names become possible. First, the maximum number of noncumulative double bonds is added after introduction of the carbonyl group(s), and any hydrogen that remains to be added is denoted as indicated hydrogen with the carbonyl group having priority over the indicated hydrogen for lower-numbered locant. Second, the prefix oxo- is used, with the hydrogenation indicated by hydro prefixes; hydrogenation is considered to have occurred before the introduction of the carbonyl group. For example,

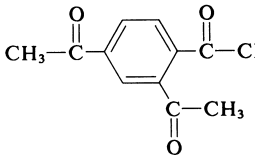


(1) 1-(*2H*)-Naphthalenone
(2) 1-Oxo-1,2-dihydronaphthalene

When another group having higher priority for citation as principal group is also present, the ketonic oxygen may be expressed by the prefix oxo-, or one can use the name of the carbonyl-containing radical, as, for example, acyl radicals and oxo-substituted radicals. Examples are



4-(4′-Oxohexyl)-1-benzoic acid

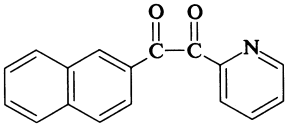


1,2,4-Triacetylbenzene

Diketones and tetraketones derived from aromatic compounds by conversion of two or four $\geq CH$ groups into keto groups, with any necessary rearrangement of double bonds to a quinonoid structure, are named by adding the suffix -quinone and any necessary affixes.

Polyketones in which two or more contiguous carbonyl groups have rings attached at each end

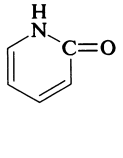
may be named (1) by the radicofunctional method or (2) by substitutive nomenclature. For example,



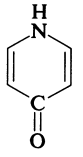
(1) 2-Naphthyl 2-pyridyl diketone
(2) 1-(2-Naphthyl)-2-(2-pyridyl)ethanedione

Some trivial names are retained: acetone (2-propanone), biacetyl (2,3-butanedione), propiophenone ($C_6H_5—CO—CH_2CH_3$), chalcone ($C_6H_5—CH{=}CH—CO—C_6H_5$), and deoxybenzoin ($C_6H_5—CH_2—CO—C_6H_5$).

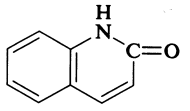
These contracted names of heterocyclic nitrogen compounds are retained as alternatives for systematic names, sometimes with indicated hydrogen. In addition, names of oxo derivatives of fully saturated nitrogen heterocycles that systematically end in -idinone are often contracted to end in -idone when no ambiguity might result. For example,



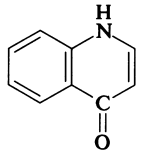
2-Pyridone
2(1*H*)-Pyridone



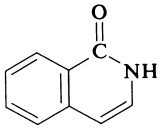
4-Pyridone
4(1*H*)-Pyridone



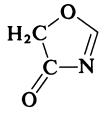
2-Quinolone
2(1*H*)-Quinolone



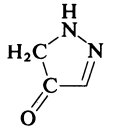
4-Quinolone
4(1*H*)-Quinolone



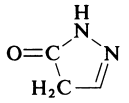
1-Isoquinolone
1(2*H*)-Isoquinolone



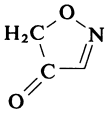
4-Oxazolone
4(5*H*)-Oxazolone



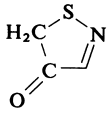
4-Pyrazolone
4(5*H*)-Pyrazolone



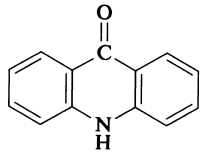
5-Pyrazolone
5(4*H*)-Pyrazolone



4-Isoxazoline
4(5*H*)-Isoxazolone



4-Thiazolone
4(5*H*)-Thiazolone



9-Acridone
9(10*H*)-Acridone

1.1.3.19 Lactones, Lactides, Lactams, and Lactims. When the hydroxy acid from which water may be considered to have been eliminated has a trivial name, the lactone is designated by substituting -olactone for -ic acid. Locants for a carbonyl group are numbered as low as possible, even before that of a hydroxyl group.

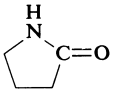
Lactones formed from aliphatic acids are named by adding -olide to the name of the nonhydroxylated hydrocarbon with the same number of carbon atoms. The suffix -olide signifies the change of $\succ CH\cdots CH_3$ into $\succ C(\cdots C{=}O)O\text{-}$.

Structures in which one or more (but not all) rings of an aggregate are lactone rings are named by placing -carbolactone (denoting the —O—CO— bridge) after the names of the structures that

remain when each bridge is replaced by two hydrogen atoms. The locant for —CO— is cited before that for the ester oxygen atom. An additional carbon atom is incorporated into this structure as compared to the -olide.

These trivial names are permitted: γ-butyrolactone, γ-valerolactone, and δ-valerolactone. Names based on heterocycles may be used for all lactones. Thus, γ-butyrolactone is also tetrahydro-2-furanone or dihydro-2(3*H*)-furanone.

Lactides, intermolecular cyclic esters, are named as heterocycles. *Lactams* and *lactims*, containing a —CO—NH— and —C(OH)═N— group, respectively, are named as heterocycles, but they may also be named with -lactam or -lactim in place of -olide. For example,



(1) 2-Pyrrolidinone
(2) 4-Butanelactam

1.1.3.20 Nitriles and Related Compounds. For acids whose systematic names end in -carboxylic acid, nitriles are named by adding the suffix -carbonitrile when the —CN group replaces the —COOH group. The carbon atom of the —CN group is excluded from the numbering of a chain to which it is attached. However, when the triple-bonded nitrogen atom is considered to replace three hydrogen atoms at the end of the main chain of an acyclic hydrocarbon, the suffix -nitrile is added to the name of the hydrocarbon. Numbering begins with the carbon attached to the nitrogen. For example, $CH_3CH_2CH_2CH_2CH_2CN$ is named (1) pentanecarbonitrile or (2) hexanenitrile.

Trivial acid names are formed by changing the endings -oic acid or -ic acid to -onitrile. For example, CH_3CN is acetonitrile. When the —CN group is not the highest priority group, the —CN group is denoted by the prefix cyano-.

In order of decreasing priority for citation of a functional class name, and the prefix for substitutive nomenclature, are the following related compounds:

Functional group	Prefix	Radicofunctional ending
—NC	Isocyano-	Isocyanide
—OCN	Cyanato-	Cyanate
—NCO	Isocyanato-	Isocyanate
—ONC	—	Fulminate
—SCN	Thiocyanato-	Thiocyanate
—NCS	Isothiocyanato-	Isothiocyanate
—SeCN	Selenocyanato-	Selenocyanate
—NCSe	Isoselenocyanato-	Isoselenocyanate

1.1.3.21 Peroxides. Compounds of the type R—O—OH are named (1) by placing the name of the radical R before the word *hydroperoxide* or (2) by use of the prefix hydroperoxy- when another parent name has higher priority. For example, C_2H_5OOH is ethyl hydroperoxide.

Compounds of the type $R^1O—OR^2$ are named (1) by placing the names of the radicals in alphabetical order before the word *peroxide* when the group —O—O— links two chains, two rings, or a ring and a chain, (2) by use of the affix dioxy to denote the bivalent group —O—O— for naming assemblies of identical units or to form part of a prefix, or (3) by use of the prefix epidioxy- when the peroxide group forms a bridge between two carbon atoms, a ring, or a ring system.

Examples are methyl propyl peroxide for $CH_3—O—O—C_3H_7$ and 2,2′-dioxydiacetic acid for $HOOC—CH_2—O—O—CH_2—COOH$.

1.1.3.22 Phosphorus Compounds. Acyclic phosphorus compounds containing only one phosphorus atom, as well as compounds in which only a single phosphorus atom is in each of several functional groups, are named as derivatives of the parent structures listed in Table 1.12. Often these

TABLE 1.12 Parent Structures of Phosphorus-Containing Compounds

Formula	Parent name	Substitutive prefix	Radicofunctional ending
H_3P	Phosphine	$H_2P—$ Phosphino-	Phosphide
H_5P	Phosphorane	$H_4P—$ Phosphoranyl-	
		$H_3P\lessdot$ Phosphoroanediyl-	
		$H_2P\lessdot\!\!\lessdot$ Phosphoranetriyl-	
H_3PO	Phosphine oxide		
H_3PS	Phosphine sulfide		
H_3PNH	Phosphine imide		
$P(OH)_3$	Phosphorous acid		Phosphite
$HP(OH)_2$	Phosphonous acid		Phosphonite
H_2POH	Phosphinous acid		Phosphinite
$P(O)(OH)_3$	Phosphoric acid	$P(O)\lessdot\!\!\lessdot$ Phosphoryl-	Phosphate(V)
$HP(O)(OH)_2$	Phosphonic acid	$HP(O)\lessdot$ Phosphonoyl-	Phosphonate
		$—P(O)OH_2$ Phosphono-	
$H_2P(O)OH$	Phosphinic acid	$H_2P(O)—$ Phosphinoyl-	Phosphinate
		$\gtrdot P(O)OH$ Phosphinoco-	
		Phosphinato-	

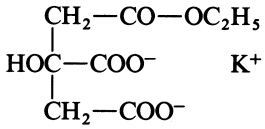
are purely hypothetical parent structures. When hydrogen attached to phosphorus is replaced by a hydrocarbon group, the derivative is named by substitution nomenclature. When hydrogen of an —OH group is replaced, the derivative is named by radicofunctional nomenclature. For example, $C_2H_5PH_2$ is ethylphosphine; $(C_2H_5)_2PH$, diethylphosphine; $CH_3P(OH)_2$, dihydroxy-methyl-phosphine or methylphosphonous acid; $C_2H_5—PO(Cl)(OH)$, ethylchlorophosphonic acid or ethylphosphonochloridic acid or hydrogen chlorodioxoethylphosphate(V); $CH_3CH(PH_2)COOH$, 2-phosphinopropionic acid; $HP(CH_2COOH)_2$, phosphinediyldiacetic acid; $(CH_3)HP(O)OH$, methylphosphinic acid or hydrogen hydridomethyldioxophosphate(V); $(CH_3O)_3PO$, trimethyl phosphate; and $(CH_3O)_3P$, trimethyl phosphite.

1.1.3.23 Salts and Esters of Acids. Neutral salts of acids are named by citing the cation(s) and then the anion, whose ending is changed from -oic to -oate or from -ic to -ate. When different acidic residues are present in one structure, prefixes are formed by changing the anion ending -ate to -ato- or -ide to -ido-. The prefix carboxylato- denotes the ionic group $—COO^-$. The phrase (metal) salt of (the acid) is permissible when the carboxyl groups are not all named as affixes.

Acid salts include the word *hydrogen* (with affixes, if appropriate) inserted between the name of the cation and the name of the anion (or word *salt*).

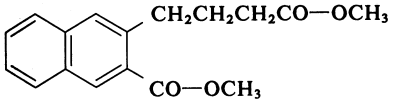
Esters are named similarly, with the name of the alkyl or aryl radical replacing the name of the

cation. Acid esters of acids and their salts are named as neutral esters, but the components are cited in the order: cation, alkyl or aryl radical, hydrogen, and anion. Locants are added if necessary. For example,



Potassium 1-ethyl hydrogen citrate

Ester groups in $R^1—CO—OR^2$ compounds are named (1) by the prefix alkoxycarbonyl- or aryloxycarbonyl- for $—CO—OR^2$ when the radical R^1 contains a substituent with priority for citation as principal group or (2) by the prefix acyloxy- for $R^1—CO—O—$ when the radical R^2 contains a substituent with priority for citation as principal group. Examples are



Methyl 3-methoxycarbonyl-2-naphthalenebutyrate

$[CH_3O—CO—CH_2CH_2\overset{+}{N}(CH_3)_3]Cl^-$ [(2-Methoxycarbonyl)ethyl]trimethylammonium chloride

$C_6H_5—CO—OCH_2CH_2COOH$ 3-Benzoyloxypropionic acid

The trivial name *acetoxy* is retained for the $CH_3—CO—O—$ group. Compounds of the type $R^2C(OR^2)_3$ are named as R^2 esters of the hypothetical ortho acids. For example, $CH_3C(OCH_3)_3$ is trimethyl orthoacetate.

1.1.3.24 Silicon Compounds. SiH_4 is called silane; its acyclic homologs are called disilane, trisilane, and so on, according to the number of silicon atoms present. The chain is numbered from one end to the other so as to give the lowest-numbered locant in radicals to the free valence or to substituents on a chain. The abbreviated form silyl is used for the radical $SiH_3—$. Numbering and citation of side chains proceed according to the principles set forth for hydrocarbon chains. Cyclic nonaromatic structures are designated by the prefix cyclo-.

When a chain or ring system is composed entirely of alternating silicon and oxygen atoms, the parent name *siloxane* is used with a multiplying affix to denote the number of silicon atoms present. The parent name *silazane* implies alternating silicon and nitrogen atoms; multiplying affixes denote the number of silicon atoms present.

The prefix sila- designates replacement of carbon by silicon in replacement nomenclature. Prefix names for radicals are formed analogously to those for the corresponding carbon-containing compounds. Thus silyl is used for $SiH_3—$, silyene for $—SiH_2—$, silylidyne for $—SiH<$, as well as trily, tetrayl, and so on for free valences(s) on ring structures.

1.1.3.25 Sulfur Compounds

Bivalent Sulfur. The prefix thio, placed before an affix that denotes the oxygen-containing group or an oxygen atom, implies the replacement of that oxygen by sulfur. Thus the suffix -thiol denotes —SH, -thione denotes —(C)═S and implies the presence of an ═S at a nonterminal carbon atom, -thioic acid denotes [(C)═S]OH ⇌ [(C)═O]SH (that is, the *O*-substituted acid and the *S*-substi-

tuted acid, respectively), -dithioc acid denotes [—C(S)]SH, and -thial denotes —(C)HS (or -carbothialdehyde denotes —CHS). When -carboxylic acid has been used for acids, the sulfur analog is named -carbothioic acid or -carbodithioic acid.

Prefixes for the groups HS— and RS— are mercapto- and alkylthio-, respectively; this latter name may require parentheses for distinction from the use of thio- for replacement of oxygen in a trivially named acid. Examples of this problem are 4-C_2H_5—C_6H_4—CSOH named *p*-ethyl(thio)benzoic acid and 4-C_2H_5—S—C_6H_4—COOH named *p*-(ethylthio)benzoic acid. When —SH is not the principal group, the prefix mercapto- is placed before the name of the parent compound to denote an unsubstituted —SH group.

The prefix thioxo- is used for naming =S in a thioketone. Sulfur analogs of acetals are named as alkylthio- or arylthio-. For example, $CH_3CH(SCH_3)OCH_3$ is 1-methoxy-1-(methylthio)ethane. Prefix forms for -carbothioic acids are hydroxy(thiocarbonyl)- when referring to the *O*-substituted acid and mercapto(carbonyl)- for the *S*-substituted acid.

Salts are formed as with oxygen-containing compounds. For example, C_2H_5—S—Na is named either sodium ethanethiolate or sodium ethyl sulfide. If mercapto- has been used as a prefix, the salt is named by use of the prefix sulfido- for —S^-.

Compounds of the type R^1—S—R^2 are named alkylthio- (or arylthio-) as a prefix to the name of R^1 or R^2, whichever is the senior.

Sulfonium Compounds. Sulfonium compounds of the type $R^1R^2R^3S^+X^-$ are named by citing in alphabetical order the radical names followed by -sulfonium and the name of the anion. For heterocyclic compounds, -ium is added to the name of the ring system. Replacement of >CH by sulfonium sulfur is denoted by the prefix thionia-, and the name of the anion is added at the end.

Organosulfur Halides. When sulfur is directly linked only to an organic radical and to a halogen atom, the radical name is attached to the word *sulfur* and the name(s) and number of the halide(s) are stated as a separate word. Alternatively, the name can be formed from R—SOH, a sulfenic acid whose radical prefix is sulfenyl-. For example, CH_3CH_2—S—Br would be named either ethylsulfur monobromide or ethanesulfenyl bromide. When another principal group is present, a composite prefix is formed from the number and substitutive name(s) of the halogen atoms in front of the syllable thio. For example, BrS—COOH is (bromothio)formic acid.

Sulfoxides. Sulfoxides, R^1—SO—R^2, are named by placing the names of the radicals in alphabetical order before the word *sulfoxide.* Alternatively, the less senior radical is named followed by sulfinyl- and concluded by the name of the senior group. For example, CH_3CH_2—SO—$CH_2CH_2CH_3$ is named either ethyl propyl sulfoxide or 1-(ethylsulfinyl)propane.

When an >SO group is incorporated in a ring, the compound is named an oxide.

Sulfones. Sulfones, R^1—SO_2—R^2, are named in an analogous manner to sulfoxides, using the word *sulfone* in place of *sulfoxide.* In prefixes, the less senior radical is followed by -sulfonyl-. When the >SO_2 group is incorporated in a ring, the compound is named as a dioxide.

Sulfur Acids. Organic oxy acids of sulfur, that is, —SO_3H, —SO_2H, and —SOH, are named sulfonic acid, sulfinic acid, and sulfenic acid, respectively. In subordinate use, the respective prefixes are sulfo-, sulfino, and sulfeno-. The grouping —SO_2—O—SO_2— or —SO—O—SO is named sulfonic or sulfinic anhydride, respectively.

Inorganic nomenclature is employed in naming sulfur acids and their derivatives in which sulfur is linked only through oxygen to the organic radical. For example, $(C_2H_5O)_2SO_2$ is diethyl sulfate and C_2H_5O—SO_2—OH is ethyl hydrogen sulfate. Prefixes *O*- and *S*- are used where necessary to denote attachment to oxygen and to sulfur, respectively, in sulfur replacement compounds. For example, CH_3—S—SO_2—ONa is sodium *S*-methyl thiosulfate.

When sulfur is linked only through nitrogen, or through nitrogen and oxygen, to the organic radical, naming is as follows: (1) *N*-substituted amides are designated as *N*-substituted derivatives of the sulfur amides and (2) compounds of the type R—NH—SO_3H may be named as *N*-substituted

sulfamic acids or by the prefix sulfoamino- to denote the group $HO_3S—NH—$. The groups —N═SO and —N═SO_2 are named sulfinylamines and sulfonylamines, respectively.

Sultones and Sultams. Compounds containing the group —SO_2—O— as part of the ring are called -sultone. The —SO_2— group has priority over the —O— group for lowest-numbered locant.

Similarly, the —SO_2—N═ group as part of a ring is named by adding -sultam to the name of the hydrocarbon with the same number of carbon atoms. The —SO_2— has priority over —N═ for lowest-numbered locant.

1.1.4 Stereochemistry

Concepts in stereochemistry, that is, chemistry in three-dimensional space, are in the process of rapid expansion. This section will deal with only the main principles. The compounds discussed will be those that have identical molecular formulas but differ in the arrangement of their atoms in space. *Stereoisomers* is the name applied to these compounds.

Stereoisomers can be grouped into three categories: (1) Conformational isomers differ from each other only in the way their atoms are oriented in space, but can be converted into one another by rotation about sigma bonds. (2) Geometric isomers are compounds in which rotation about a double bond is restricted. (3) Configurational isomers differ from one another only in configuration about a chiral center, axis, or plane. In subsequent structural representations, a broken line denotes a bond projecting behind the plane of the paper and a wedge denotes a bond projecting in front of the plane of the paper. A line of normal thickness denotes a bond lying essentially in the plane of the paper.

1.1.4.1 Conformational Isomers. A molecule in a conformation into which its atoms return spontaneously after small displacements is termed a *conformer*. Different arrangements of atoms that can be converted into one another by rotation about single bonds are called *conformational isomers* (see Fig. 1.1). A pair of conformational isomers can be but do not have to be mirror images of each other. When they are not mirror images, they are called *diastereomers.*

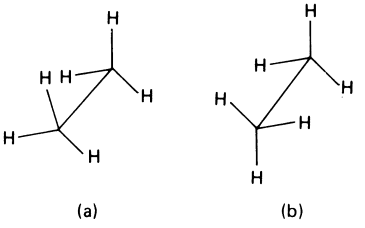


FIGURE 1.1 Conformations of ethane. (*a*) Eclipsed; (*b*) staggered.

Acyclic Compounds. Different conformations of acyclic compounds are best viewed by construction of ball-and-stick molecules or by use of Newman projections (see Fig. 1.2). Both types of representations are shown for ethane. Atoms or groups that are attached at opposite ends of a single bond should be viewed along the bond axis. If two atoms or groups attached at opposite ends of the bond appear one directly behind the other, these atoms or groups are described as eclipsed. That portion of the molecule is described as being in the eclipsed conformation. If not eclipsed, the atoms

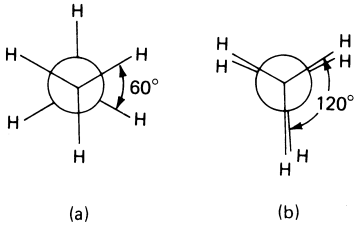


FIGURE 1.2 Newman projections for ethane. (*a*) Staggered; (*b*) eclipsed.

or groups and the conformation may be described as staggered. Newman projections show these conformations clearly.

Certain physical properties show that rotation about the single bond is not quite free. For ethane there is an energy barrier of about 3 kcal · mol^{-1} (12 kJ · mol^{-1}).The potential energy of the molecule is at a minimum for the staggered conformation, increases with rotation, and reaches a maximum at the eclipsed conformation. The energy required to rotate the atoms or groups about the carbon-carbon bond is called *torsional energy*. Torsional strain is the cause of the relative instability of the eclipsed conformation or any intermediate skew conformations.

In butane, with a methyl group replacing one hydrogen on each carbon of ethane, there are several different staggered conformations (see Fig. 1.3). There is the *anti*-conformation in which the methyl groups are as far apart as they can be (dihedral angle of 180°). There are two *gauche* conformations in which the methyl groups are only 60° apart; these are two nonsuperimposable mirror images of each other. The *anti*-conformation is more stable than the *gauche* by about 0.9 kcal · mol^{-1} (4 kJ · mol^{-1}). Both are free of torsional strain. However, in a *gauche* conformation the methyl groups are closer together than the sum of their van der Waals' radii. Under these conditions van der Waals' forces are repulsive and raise the energy of conformation. This strain can affect not only the relative stabilities of various staggered conformations but also the heights of the energy barriers

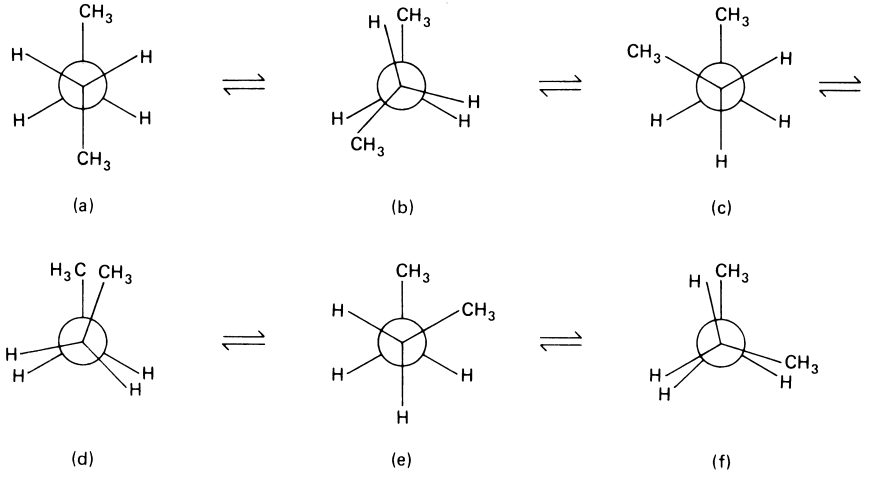


FIGURE 1.3 Conformations of butane. (*a*) *Anti*-staggered; (*b*) eclipsed; (*c*) *gauche*-staggered; (*d*) eclipsed; (*e*) *gauche*-staggered; (*f*) eclipsed. (Eclipsed conformations are slightly staggered for convenience in drawing; actually they are superimposed.)

between them. The energy maximum (estimated at 4.8 to 6.1 kcal · mol^{-1} or 20 to 25 kJ · mol^{-1}) is reached when two methyl groups swing past each other (the eclipsed conformation) rather than past hydrogen atoms.

Cyclic Compounds. Although cyclic aliphatic compounds are often drawn as if they were planar geometric figures (a triangle for cyclopropane, a square for cyclobutane, and so on), their structures are not that simple. Cyclopropane does possess the maximum angle strain if one considers the difference between a tetrahedral angle (109.5°) and the 60° angle of the cyclopropane structure. Nevertheless the cyclopropane structure is thermally quite stable. The highest electron density of the carbon-carbon bonds does not lie along the lines connecting the carbon atoms. Bonding electrons lie principally outside the triangular internuclear lines and result in what is known as *bent bonds* (see Fig. 1.4).

Cyclobutane has less angle strain than cyclopropane (only 19.5°). It is also believed to have some bent-bond character associated with the carbon-carbon bonds. The molecule exists in a nonplanar conformation in order to minimize hydrogen-hydrogen eclipsing strain.

Cyclopentane is nonplanar, with a structure that resembles an envelope (see Fig. 1.5). Four of the carbon atoms are in one plane, and the fifth is out of that plane. The molecule is in continual motion so that the out-of-plane carbon moves rapidly around the ring.

The 12 hydrogen atoms of cyclohexane do not occupy equivalent positions. In the chair conformation six hydrogen atoms are perpendicular to the average plane of the molecule and six are directed outward from the ring, slightly above or below the molecular plane (see Fig. 1.6). Bonds which are perpendicular to the molecular plane are known as *axial bonds*, and those which extend outward

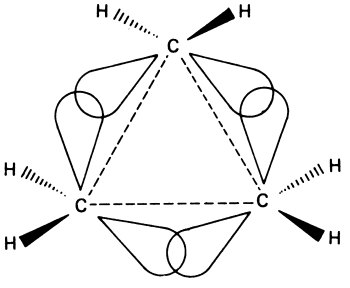


FIGURE 1.4 The bent bonds ("tear drops") of cyclopropane.

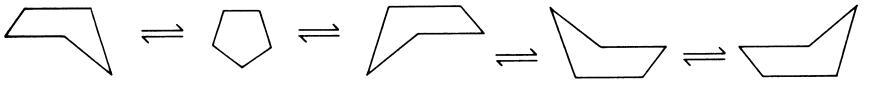


FIGURE 1.5 The conformations of cyclopentane.

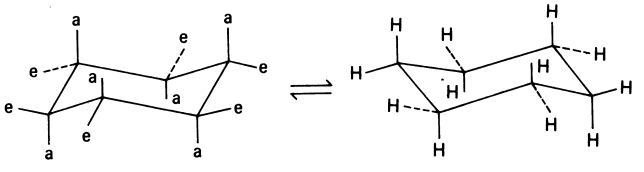


FIGURE 1.6 The two chair conformations of cyclohexane; *a* = axial hydrogen atom and *e* = equatorial hydrogen atom.

from the ring are known as *equatorial bonds.* The three axial bonds directed upward originate from alternate carbon atoms and are parallel with each other; a similar situation exists for the three axial bonds directed downward. Each equatorial bond is drawn so as to be parallel with the ring carbon-carbon bond once removed from the point of attachment to that equatorial bond. At room temperature, cyclohexane is interconverting rapidly between two chair conformations. As one chair form converts to the other, all the equatorial hydrogen atoms become axial and all the axial hydrogens become equatorial. The interconversion is so rapid that all hydrogen atoms on cyclohexane can be considered equivalent. Interconversion is believed to take place by movement of one side of the chair structure to produce the twist boat, and then movement of the other side of the twist boat to give the other chair form. The chair conformation is the most favored structure for cyclohexane. No angle strain is encountered since all bond angles remain tetrahedral. Torsional strain is minimal because all groups are staggered.

In the boat conformation of cyclohexane (Fig. 1.7) eclipsing torsional strain is significant, although no angle strain is encountered. Nonbonded interaction between the two hydrogen atoms across the ring from each other (the "flagpole" hydrogens) is unfavorable. The boat conformation is about 6.5 kcal $\cdot$ mol^{-1} (27 kJ $\cdot$ mol^{-1}) higher in energy than the chair form at 25°C.

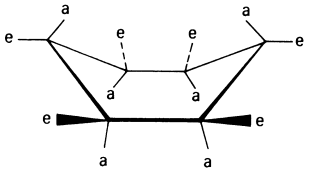


FIGURE 1.7 The boat conformation of cyclohexane. *a* = axial hydrogen atom and *e* = equatorial hydrogen atom.

FIGURE 1.8 Twist-boat conformation of cyclohexane.

A modified boat conformation of cyclohexane, known as the twist boat (Fig. 1.8), or skew boat, has been suggested to minimize torsional and nonbounded interactions. This particular conformation is estimated to be about 1.5 kcal $\cdot$ mol^{-1} (6 kJ $\cdot$ mol^{-1}) lower in energy than the boat form at room temperature.

The medium-size rings (7 to 12 ring atoms) are relatively free of angle strain and can easily take a variety of spatial arrangements. They are not large enough to avoid all nonbonded interactions between atoms.

Disubstituted cyclohexanes can exist as *cis-trans* isomers as well as axial-equatorial conformers. Two isomers are predicted for 1,4-dimethylcyclohexane (see Fig. 1.9). For the *trans* isomer the diequatorial conformer is the energetically favorable form. Only one *cis* isomer is observed, since the two conformers of the *cis* compound are identical. Interconversion takes place between the conformational (equatorial-axial) isomers but not configurational (*cis-trans*) isomers.

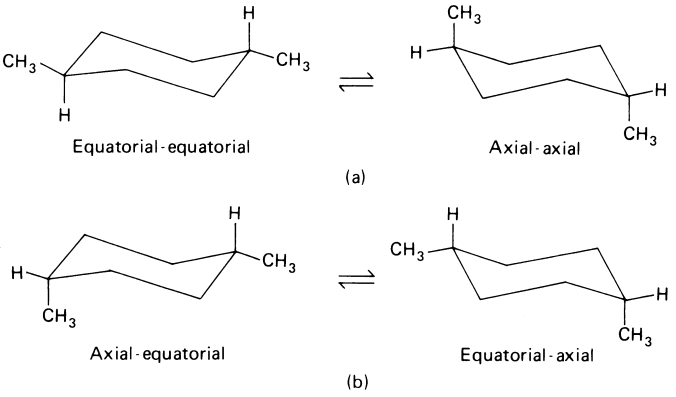


FIGURE 1.9 Two isomers of 1,4-dimethylcyclohexane. (*a*) *Trans* isomer; (*b*) *cis* isomer.

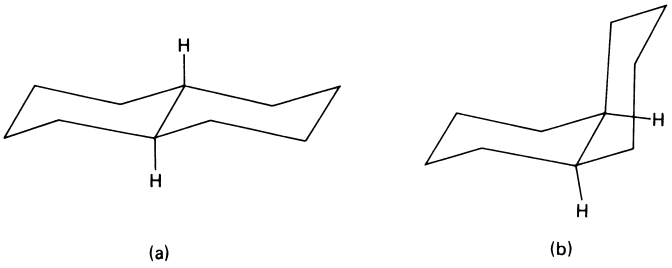


FIGURE 1.10 Two isomers of decahydronaphthalene, or bicyclo[4.4.0]decane. (*a*) *Trans* isomer; (*b*) *cis* isomer.

The bicyclic compound decahydronaphthalene, or bicyclo[4.4.0]decane, has two fused six-membered rings. It exists in *cis* and *trans* forms (see Fig. 1.10), as determined by the configurations at the bridgehead carbon atoms. Both *cis*- and *trans*-decahydronaphthalene can be constructed with two chair conformations.

1.1.4.2 Geometrical Isomerism. Rotation about a carbon-carbon double bond is restricted because of interaction between the *p* orbitals which make up the pi bond. Isomerism due to such restricted rotation about a bond is known as *geometric isomerism.* Parallel overlap of the *p* orbitals of each carbon atom of the double bond forms the molecular orbital of the pi bond. The relatively large barrier to rotation about the pi bond is estimated to be nearly 63 kcal · mol^{-1} (263 kJ · mol^{-1}).

When two different substituents are attached to each carbon atom of the double bond, *cis-trans* isomers can exist. In the case of *cis*-2-butene (Fig. 1.11*a*), both methyl groups are on the same side of the double bond. The other isomer has the methyl groups on opposite sides and is designated as *trans*-2-butene (Fig. 1.11*b*). Their physical properties are quite different. Geometric isomerism can also exist in ring systems; examples were cited in the previous discussion on conformational isomers.

For compounds containing only double-bonded atoms, the reference plane contains the double-bonded atoms and is perpendicular to the plane containing these atoms and those directly attached to them. It is customary to draw the formulas so that the reference plane is perpendicular to that of

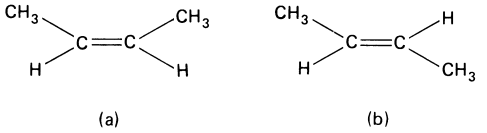


FIGURE 1.11 Two isomers of 2-butene. (*a*) *Cis* isomer, bp 3.8°C, mp −138.9°C, dipole moment 0.33 D; (*b*) *trans* isomer, bp 0.88°C, mp −105.6°C, dipole moment 0 D.

the paper. For cyclic compounds the reference plane is that in which the ring skeleton lies or to which it approximates. Cyclic structures are commonly drawn with the ring atoms in the plane of the paper.

1.1.4.3 Sequence Rules for Geometric Isomers and Chiral Compounds. Although *cis* and *trans* designations have been used for many years, this approach becomes useless in complex systems. To eliminate confusion when each carbon of a double bond or a chiral center is connected to different groups, the Cahn, Ingold, and Prelog system for designating configuration about a double bond or a chiral center has been adopted by IUPAC. Groups on each carbon atom of the double bond are assigned a first (1) or second (2) priority. Priority is then compared at one carbon relative to the other. When both first priority groups are on the *same side* of the double bond, the configuration is designated as *Z* (from the German *zusammen*, "together"), which was formerly *cis.* If the first priority groups are on *opposite sides* of the double bond, the designation is *E* (from the German *entgegen*, "in opposition to"), which was formerly *trans.* (See Fig. 1.12.)

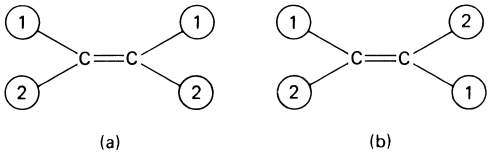
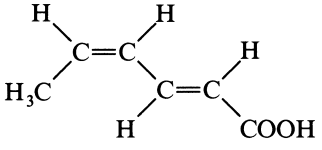


FIGURE 1.12 Configurations designated by priority groups. (*a*) *Z* (*cis*); (*b*) *E* (*trans*).

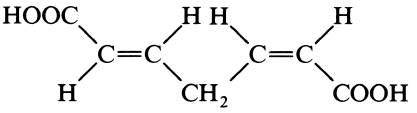
When a molecule contains more than one double bond, each *E* or *Z* prefix has associated with it the lower-numbered locant of the double bond concerned. Thus (see also the rules that follow)



(2*E*,4*Z*)-2,4-Hexadienoic acid

When the sequence rules permit alternatives, preference for lower-numbered locants and for inclusion in the principal chain is allotted as follows in the order stated: *Z* over *E* groups and *cis* over *trans* cyclic groups. If a choice is still not attained, then the lower-numbered locant for such a preferred

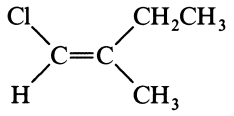
group at the first point of difference is the determining factor. For example,



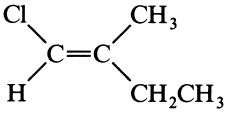
(2*Z*,5*E*)-2,5-Heptadienedioic acid

Rule 1. Priority is assigned to atoms on the basis of atomic number. Higher priority is assigned to atoms of higher atomic number. If two atoms are isotopes of the same element, the atom of higher mass number has the higher priority. For example, in 2-butene, the carbon atom of each methyl group receives first priority over the hydrogen atom connected to the same carbon atom. Around the asymmetric carbon atom in chloroiodomethanesulfonic acid, the priority sequence is I, Cl, S, H. In 1-bromo-1-deuteroethane, the priority sequence is Cl, C, D, H.

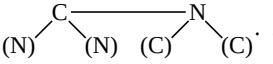
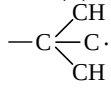
Rule 2. When atoms attached directly to a double-bonded carbon have the same priority, the second atoms are considered and so on, if necessary, working outward once again from the double bond or chiral center. For example, in 1-chloro-2-methylbutene, in CH_3 the second atoms are H, H, H and in CH_2CH_3 they are C, H, H. Since carbon has a higher atomic number than hydrogen, the ethyl group has the next highest priority after the chlorine atom.



(*Z*)-1-Chloro-2-methylbutene



(*E*)-1-Chloro-2-methylbutene

Rule 3. When groups under consideration have double or triple bonds, the multiple-bonded atom is replaced conceptually by two or three single bonds to that same kind of atom. Thus, =A is considered to be equivalent to two A's, or  and ≡A equals . However, a real  has priority over =A; likewise a real has priority over ≡A. Actually, both atoms of a multiple bond are duplicated, or triplicated, so that C=O is treated as  , that is  and  , and C≡N is treated as  . A phenyl carbon becomes  . Only the double-bonded atoms themselves are duplicated, not the atoms or groups attached to them. The duplicated atoms (or phantom atoms) may be considered as carrying atomic number zero. For example, among the groups OH, CHO, CH_2OH, and H, the OH group has the highest priority, and the C(O, O, H) of CHO takes priority over the C(O, H, H) of CH_2OH.

1.1.4.4 Chirality and Optical Activity. A compound is chiral (the term *dissymmetric* was formerly used) if it is not superimposable on its mirror image. A chiral compound does not have a plane of symmetry. Each chiral compound possesses one (or more) of three types of chiral element, namely, a chiral center, a chiral axis, or a chiral plane.

Chiral Center. The chiral center, which is the chiral element most commonly met, is exemplified by an asymmetric carbon with a tetrahedral arrangement of ligands about the carbon. The ligands comprise four different atoms or groups. One "ligand" may be a lone pair of electrons; another, a phantom atom of atomic number zero. This situation is encountered in sulfoxides or with a nitrogen atom. Lactic acid is an example of a molecule with an asymmetric (chiral) carbon. (See Fig. 1.13b.)

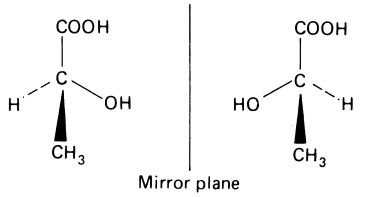
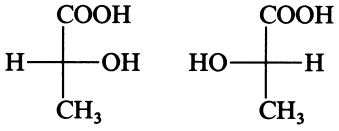


FIGURE 1.13 Asymmetric (chiral) carbon in the lactic acid molecule.

A simpler representation of molecules containing asymmetric carbon atoms is the Fischer projection, which is shown here for the same lactic acid configurations. A Fischer projection involves



drawing a cross and attaching to the four ends the four groups that are attached to the asymmetric carbon atom. The asymmetric carbon atom is understood to be located where the lines cross. The horizontal lines are understood to represent bonds coming toward the viewer out of the plane of the paper. The vertical lines represent bonds going away from the viewer behind the plane of the paper as if the vertical line were the side of a circle. The principal chain is depicted in the vertical direction; the lowest-numbered (locant) chain member is placed at the top position. These formulas may be moved sideways or rotated through 180° in the plane of the paper, but they may not be removed from the plane of the paper (i.e., rotated through 90°). In the latter orientation it is essential to use thickened lines (for bonds coming toward the viewer) and dashed lines (for bonds receding from the viewer) to avoid confusion.

Enantiomers. Two nonsuperimposable structures that are mirror images of each other are known as *enantiomers.* Enantiomers are related to each other in the same way that a right hand is related to a left hand. Except for the direction in which they rotate the plane of polarized light, enantiomers are identical in all physical properties. Enantiomers have identical chemical properties except in their reactivity toward optically active reagents.

Enantiomers rotate the plane of polarized light in opposite directions but with equal magnitude. If the light is rotated in a clockwise direction, the sample is said to be dextrorotatory and is designed as (+). When a sample rotates the plane of polarized light in a counterclockwise direction, it is said to be levorotatory and is designed as (−). Use of the designations *d* and *l* is discouraged.

Specific Rotation. Optical rotation is caused by individual molecules of the optically active compound. The amount of rotation depends upon how many molecules the light beam encounters in passing through the tube. When allowances are made for the length of the tube that contains the sample and the sample concentration, it is found that the amount of rotation, as well as its direction, is a characteristic of each individual optically active compound.

Specific rotation is the number of degrees of rotation observed if a 1-dm tube is used and the compound being examined is present to the extent of 1 g per 100 mL. The density for a pure liquid replaces the solution concentration.

$$\text{Specific rotation} = [\alpha] = \frac{\text{observed rotation (degrees)}}{\text{length (dm)} \times \text{(g/100 mL)}}$$

The temperature of the measurement is indicated by a superscript and the wavelength of the light employed by a subscript written after the bracket; for example, $[\alpha]_{590}^{20}$ implies that the measurement was made at 20°C using 590-nm radiation.

Optically Inactive Chiral Compounds. Although chirality is a necessary prerequisite for optical activity, chiral compounds are not necessarily optically active. With an equal mixture of two enantiomers, no net optical rotation is observed. Such a mixture of enantiomers is said to be *racemic* and is designated as (±) and not as *dl*. Racemic mixtures usually have melting points higher than the melting point of either pure enantiomer.

A second type of optically inactive chiral compounds, *meso* compounds, will be discussed in the next section.

Multiple Chiral Centers. The number of stereoisomers increases rapidly with an increase in the number of chiral centers in a molecule. A molecule possessing two chiral atoms should have four optical isomers, that is, four structures consisting of two pairs of enantiomers. However, if a compound has two chiral centers but both centers have the same four substituents attached, the total number of isomers is three rather than four. One isomer of such a compound is not chiral because it is identical with its mirror image; it has an internal mirror plane. This is an example of a diastereomer. The achiral structure is denoted as a *meso* compound. Diastereomers have different physical and chemical properties from the optically active enantiomers. Recognition of a plane of symmetry is usually the easiest way to detect a *meso* compound. The stereoisomers of tartaric acid are examples of compounds with multiple chiral centers (see Fig. 1.14), and one of its isomers is a *meso* compound.

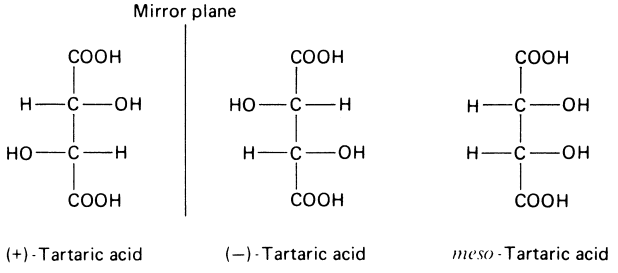


FIGURE 1.14 Isomers of tartaric acid.

When the asymmetric carbon atoms in a chiral compound are part of a ring, the isomerism is more complex than in acyclic compounds. A cyclic compound which has two different asymmetric carbons with different sets of substituent groups attached has a total of $2^2 = 4$ optical isomers: an enantiometric pair of *cis* isomers and an enantiometric pair of *trans* isomers. However, when the two asymmetric centers have the same set of substituent groups attached, the *cis* isomer is a *meso* compound and only the *trans* isomer is chiral. (See Fig. 1.15.)

Torsional Asymmetry. Rotation about single bonds of most acyclic compounds is relatively free at ordinary temperatures. There are, however, some examples of compounds in which nonbonded

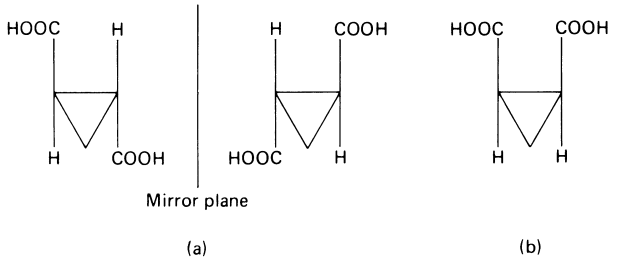


FIGURE 1.15 Isomers of cyclopropane-1,2-dicarboxylic acid. (*a*) *Trans* isomer; (*b*) *meso* isomer.

interactions between large substituent groups inhibit free rotation about a sigma bond. In some cases these compounds can be separated into pairs of enantiomers.

A *chiral axis* is present in chiral biaryl derivatives. When bulky groups are located at the *ortho* positions of each aromatic ring in biphenyl, free rotation about the single bond connecting the two rings is inhibited because of torsional strain associated with twisting rotation about the central single bond. Interconversion of enantiomers is prevented (see Fig. 1.16).

For compounds possessing a chiral axis, the structure can be regarded as an elongated tetrahedron to be viewed along the axis. In deciding upon the absolute configuration it does not matter from which end it is viewed; the nearer pair of ligands receives the first two positions in the order of precedence (see Fig. 1.17). For the meaning of (*S*), see the discussion under Absolute Configuration on p. 1.49.

A *chiral plane* is exemplified by the plane containing the benzene ring and the bromine and oxygen atoms in the chiral compound shown in Fig. 1.18. Rotation of the benzene ring around the oxygen-to-ring single bonds is inhibited when *x* is small (although no critical size can be reasonably established).

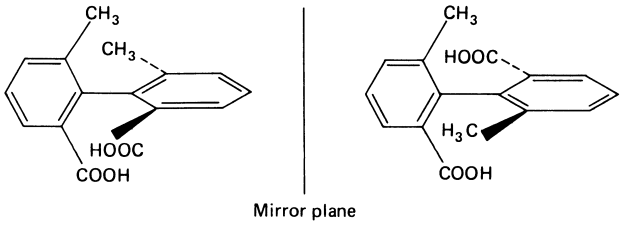


FIGURE 1.16 Isomers of biphenyl compounds with bulky groups attached at the *ortho* positions.

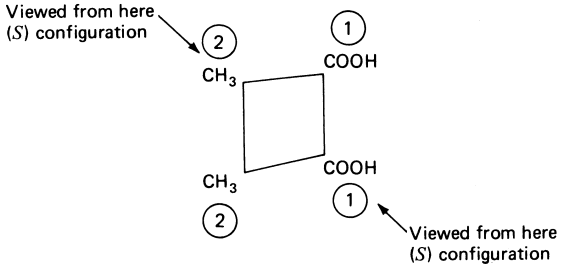


FIGURE 1.17 Example of a chiral axis.

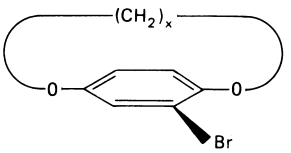


FIGURE 1.18 Example of a chiral plane.

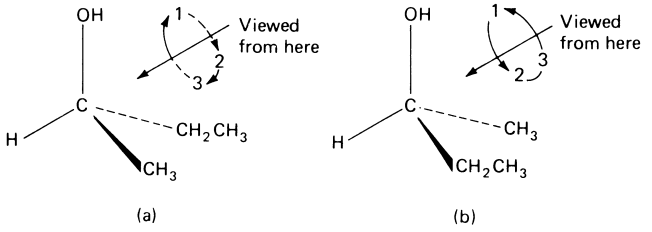


FIGURE 1.19 Viewing angle as a means of designating the absolute configuration of compounds with a chiral axis. (*a*) (*R*)-2-Butanol (sequence clockwise); (*b*) (*S*)-2-butanol (sequence counterclockwise).

Absolute Configuration. The terms absolute stereochemistry and absolute configuration are used to describe the three-dimensional arrangement of substituents around a chiral element. A general system for designating absolute configuration is based upon the priority system and sequence rules. Each group attached to a chiral center is assigned a number, with number one the highest-priority group. For example, the groups attached to the chiral center of 2-butanol (see Fig. 1.19) are assigned these priorities: 1 for OH, 2 for CH_2CH_3, 3 for CH_3, and 4 for H. The molecule is then viewed from the side opposite the group of lowest priority (the hydrogen atom), and the arrangement of the remaining groups is noted. If, in proceeding from the group of highest priority to the group of second priority and thence to the third, the eye travels in a clockwise direction, the configuration is specified *R* (from the Latin *rectus*, "right"); if the eye travels in a counterclockwise direction, the configuration is specified *S* (from the Latin *sinister*, "left"). The complete name includes both configuration and direction of optical rotation, as for example, (*S*)-(+)-2-butanol.

The relative configurations around the chiral centers of many compounds have been established. One optically active compound is converted to another by a sequence of chemical reactions which are stereospecific; that is, each reaction is known to proceed spatially in a specific way. The configuration of one chiral compound can then be related to the configuration of the next in sequence. In order to establish absolute configuration, one must carry out sufficient stereospecific reactions to relate a new compound to another of known absolute configuration. Historically the configuration of D-(+)-2,3-dihydroxypropanal has served as the standard to which all configuration has been compared. The absolute configuration assigned to this compound has been confirmed by an X-ray crystallographic technique.

1.1.5 *Chemical Abstracts* Indexing System

When compounds of complex structure are considered, the number of name possibilities grows rapidly. To avoid having index entries for all possible names, Chemical Abstracts Service has developed what might be called the principle of inversion. The indexing system employs inverted

entries to bring together related compounds in an alphabetically arranged index. The *index heading parent* from the Chemical Substance Index appears in the Formula Index in lightface before the "comma of inversion." The *substituents* follow the "comma of inversion" in alphabetical order. Any *name modification* appears on a separate line. If necessary, the chemical description is completed by citation of an associated ion, a functional derivative, a "salt with" or "compound with" term, and/or a stereochemical descriptor.

Quite naturally there is a certain amount of arbitrariness in this system, although the IUPAC nomenclature is followed. The preferred *Chemical Abstracts* index names for chemical substances have been, with very few exceptions, continued unchanged (since 1972) as set forth in the *Ninth Collective Index Guide* and in a journal article.* Any revisions appear in the updated *Index Guide;* new editions appear at 18-month intervals. Appendix VI is of particular interest to chemists. Reprints of the Appendix may be purchased from Chemical Abstracts Service, Marketing Division, P.O. Box 3012, Columbus, Ohio 43210.

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* *J. Chem. Doc.* **14**(1):3–15 (1974).

TABLE 1.13 Names and Formulas of Organic Radicals

For more comprehensive lists, see the various lists of radicals given in the subject indexes of the annual and decennial indexes of Chemical Abstracts.

Name	Formula	Name	Formula
Acenaphthenyl	$C_{12}H_9$—	Azido	N_3—
Acenaphthenylene	—$C_{12}H_8$—	Azino	=N—N=
Acenaphthenylidene	$C_{12}H_8$=	Azo	—N=N—
Acetamido	CH_3—CO—NH—	Azoxy	—N(O)—N—
Acetimidoyl	CH_3C(=NH)—	Azulenyl	$C_{10}H_7$—
Acetoacetyl	CH_3—CO—CH_2—CO—	Benzamido	C_6H_5—CO—NH—
Acetohydrazonoyl	CH_3—C(=NNH_2)—	Benzeneazo	C_6H_5—N=N—
Acetohydroximoyl	CH_3—C(=NOH)—	Benzeneazoxy	C_6H_5—N_2O—
Acetonyl	CH_3—CO—CH_2—	1,2-Benzenedicarbonyl, *see* Phthaloyl	
Acetonylidene	CH_3—CO—CH=		
Acetoxy	CH_3—CO—O—	1,3-Benzenedicarbonyl (*or isophthaloyl*)	—CO—C_6H_4—CO— (*m*-)
Acetyl (*not ethanoyl*)	CH_3—CO—		
Acetylamino	CH_3—CO—NH—	1,4-Benzenedicarbonyl (*or terephthaloyl*)	—CO—C_6H_4—CO— (*p*-)
Acetylhydrazino	CH_3—CO—NH—NH—		
Acetylimino	CH_3—CO—N=	Benzenesulfinyl	C_6H_5—SO—
Acridinyl (*from acridine*)	$NC_{13}H_8$—	Benzenesulfonamido	C_6H_5—SO_2—NH—
Acroyloyl (*or propenoyl*)	CH_2=CH—CO—	Benzenesulfonyl	C_6H_5—SO_2—
Adipoyl (*or hexanedioyl*)	—CO—$[CH_2]_4$—CO—	Benzenesulfonylamino	C_6H_5—SO_2—NH—
Alanyl	CH_3—CH(NH_2)—CO—	Benzenetriyl	C_6H_3—
β-Alanyl	H_2N—CH_2—CH_2—CO—	Benzhydryl (*or diphenylmethyl*)	$(C_6H_5)_2$CH—
Allyl (*or 2-propenyl*)	CH_2=CH—CH_2—	Benzidino	*p*-H_2N—C_6H_4—C_6H_4—NH—
Allylidene	CH_2=CH—CH=		
Allyloxy	CH_2=CH—CH_2—O—		
Amidino	H_2N—C(=NH)—	Benziloyl (*or 2-hydroxy-2,2-diphenylethanoyl*)	$(C_6H_5)_2$C(OH)—CO—
Amino	H_2N—		
Aminomethyleneamino	H_2N—CH=N—	Benzimidazolyl	$N_2C_7H_5$—
Aminooxy	H_2N—O—	Benzimidoyl	C_6H_5—C(=NH)—
Ammonio	^+H_3N—	Benzofuranyl	OC_8H_5—
Amyl, *see* Pentyl		Benzopyranyl	OC_9H_7—
Anilino	C_6H_5—NH—	Benzoquinonyl (1,2- or 1,4-)	(O=)$_2C_6H_3$—
Anisidino (*o*-, *m*-, *or p*-)	CH_3O—C_6H_4—NH—	Benzo[*b*]thienyl	SC_8H_5—
Anisoyl (*o*-, *m*-, *or p*-; *or methoxybenzoyl*)	CH_3O—C_6H_4—CO—	Benzoyl	C_6H_5—CO—
		Benzoylamino	C_6H_5—CO—NH—
		Benzoylhydrazino	C_6H_5—CO—NH—NH—
Anthraniloyl	*o*-NH_2—C_6H_4—CO—	Benzoylimino	C_6H_5—CO—N=
Anthryl (*from anthracene*)	$C_{14}H_9$—	Benzoyloxy	C_6H_5—CO—O—
Anthrylene	—$C_{14}H_8$—	Benzyl	C_6H_5—CH_2—
Arginyl	H_2N—C(=NH)—NH—$[CH_2]_3$—CH(NH)—CO—	Benzylidene	C_6H_5—CH=
		Benzylidyne	C_6H_5—C≡
		Benzyloxy	C_6H_5—CH_2—O—
Asparaginyl	H_2N—CO—CH_2—CH(NH_2)—CO—	Benzyloxycarbonyl	C_6H_5—CH_2—O—CO—
		Benzylthio	C_6H_5—CH_2—S—
Aspartoyl	—CO—CH_2—CH(NH_2)—CO—	Biphenylenyl	$C_{12}H_7$—
		Biphenylyl	C_6H_5—C_6H_4—
α-Aspartyl	HO_2C—$CH_2CH(NH_2)$—	Bornenyl	$C_{10}H_{15}$—
Atropoyl (*or 2-phenylpropenoyl*)	C_6H_5—C(=CH_2)—CO—	Bornyl (*not camphyl or bornylyl*)	$C_{10}H_{17}$—
Azelaoyl, *see* Nonanedioyl		Bromo	Br—
		Bromoformyl	Br—CO—

TABLE 1.13 Names and Formulas of Organic Radicals (*Continued*)

Name	Formula
Bromonio	$^{+}HBr-$
Butadienyl (1,3- shown)	$CH_2=CH-CH=CH-$
Butanedioyl, *see* Succinyl	
Butanediylidene	$=CH-CH_2-CH_2-CH=$
Butanediylidyne	$\equiv C-CH_2-CH_2-C\equiv$
Butanoyl, *see* Butyryl	
cis-Butenedioyl, *see* Maleoyl	
trans-Butenedioyl, *see* Fumaroyl Butenoyl, *see* Crotonoyl and Isocrotonoyl	
1-Butenyl	$CH_3-CH_2-CH=CH-$
2-Butenyl (*not crotyl*)	$CH_3-CH=CH-CH_2-$
2-Butenylene	$-CH_2-CH=CH-CH_2-$
Butenylidene (*2- shown*)	$CH_3CH=CH-CH=$
Butenylidyne (*2- shown*)	$CH_3-CH=CH-C\equiv$
Butoxy	$CH_3-[CH_2]_3-O-$
sec-Butoxy (*unsubstituted only*)	$C_2H_5-CH(CH_3)-O-$
tert-Butoxy (*unsubstituted only*)	$(CH_3)_3C-O-$
Butyl	$CH_3-[CH_2]_3-$ or C_4H_9-
sec-Butyl (*unsubstituted only*)	$C_2H_5-CH(CH_3)-$
tert-Butyl (*unsubstituted only*)	$(CH_3)_3C-$
Butylidene	$CH_3-CH_2-CH_2-CH=$
sec-Butylidene (*unsubstituted only*)	$C_2H_5C(CH_3)=$
Butylidyne	$CH_3-[CH_2]_2-C\equiv$
Butyryl (*or butanoyl*)	$CH_3-CH_2-CH_2-CO-$
Camphoroyl	$C_{10}H_{14}O_2-$
Carbamoyl	H_2N-CO-
Carbazolyl	$NC_{12}H_8-$
Carbazoyl	$H_2N-NH-CO-$
Carbonimidoyl	$-C(=NH)-$
Carbonohydrazido (*preferred to carbohydazido or carbazido*)	$H_2N-NH-CO-NH-NH-$
Carbonyl	$-CO-$ or $=C(O)$
Carbonyldioxy	$-O-CO-O-$
Carboxy	HO_2C-
Carboxylato	$-O_2C-$
Chloro	$Cl-$
Chlorocarbonyl, *see* Chloroformyl	
Chloroformyl	$Cl-C(O)-$
Chlorosyl	$OCl-$
Chlorothio	$ClS-$
Chloryl	O_2Cl-

Name	Formula
Cinnamoyl (*or 3-phenylpropenoyl*)	$C_6H_5-CH=CH-CO$
Cinnamyl	$C_6H_5-CH=CH-CH_2-$
Cinnamylidene	$C_6H_5-CH=CH-CH=$
Citraconoyl (*unsubstituted only*)	$HC-CO-$ ‖ $CH_3-C-CO-$
Crotonoyl	$CH_3-CH=CH-CO-$ (*trans*)
Crotyl, *see* 2-Butenyl	
Cumenyl (*o-, m-, or p-*)	$(CH_3)_2CH-C_6H_4-$
Cyanato	$NCO-$
Cyano	$NC-$
Cyclobutyl	C_4H_7-
Cycloheptyl	$C_7H_{13}-$
Cyclohexadienyl (2,4- shown)	$CH=CH-CH-$ | | $CH=CH-CH_2$
Cyclohexadienylidene (2,4- shown)	$CH-CH_2-C$ ‖ | $CH-CH=CH$
Cyclohexanecarbonyl	$C_6H_{11}-CO-$
Cyclohexanecarbothioyl	$C_6H_{11}-CS-$
Cyclohexanecarboxamido	$C_6H_{11}-CO-NH-$
Cyclohexanecarboximidoyl	$C_6H_{11}-C(=NH)-$
Cyclohexenyl	C_6H_9-
2-Cyclohexenylidene	$CH=CH-C$ | | $H_2C-CH_2-CH_2$
Cyclohexyl	$C_6H_{11}-$
Cyclohexylcarbonyl	$C_6H_{11}-CO-$
Cyclohexylene	$-C_6H_{10}-$
Cyclohexylidene	CH_2-CH_2-C | | $CH_2-CH_2-CH_2$
Cyclohexylthiocarbonyl	$C_6H_{11}-CS-$
Cyclopentadienyl	C_5H_5-
Cyclopentadienylidene	$CH=CH-CH=CH-C=$
Cyclopenta[*a*]phenanthryl	$C_{17}H_{17}-$
1,2-Cyclopentenophenanthryl	$C_{17}H_{11}-$
Cyclopentenyl	C_5H_7-
Cyclopentyl	C_5H_9-
Cyclopentylene	$-C_5H_8-$
Cyclopropyl	C_3H_5-
Cysteinyl	$HS-CH_2-CH(NH_2)-CO-$
Cystyl	$-CO-CH(NH_2)-CH_2-S-S-CH_2-CH(NH_2)-CO-$
Decanedioyl	$-CO-[CH_2]_8-CO-$
Decanoyl	$CH_3-[CH_2]_8-CO-$
Decyl	$CH_3-[CH_2]_9-$
Diacetoxyiodo	$(CH_3-CO-O)_2I-$
Diacetylamino	$(CH_3-CO)_2N-$
Diaminomethyleneamino	$(NH_2)_2C=N-$

TABLE 1.13 Names and Formulas of Organic Radicals (*Continued*)

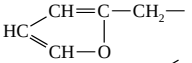
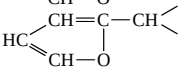
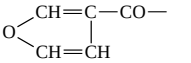
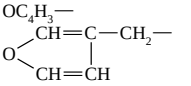
Name	Formula	Name	Formula
Diazo	$=N_2$	Fluorenyl	$C_{13}H_9-$
Diazoamino	$-N=N-NH-$	Fluoro	$F-$
Dibenzoylamino	$(C_6H_5-CO)_2N-$	Fluoroformyl	$F-CO-$
Dichloroiodo	Cl_2I-	Formamido	$OCH-NH-$
Diethylamino	$(C_2H_5)_2N-$	Formimidoyl	$CH(=NH)-$
3,4-Dihydroxybenzoyl, *see* Protocatechuoyl		Formyl (*not methanoyl*)	$OCH-$ or $-C(O)H$
		Formylamino	$H-CO-NH-$
2,3-Dihydroxybutanedioyl, *see* Tartaroyl		Formylimino	$H-CO-N=$
		Formyloxy	$H-CO-O-$
Dihydroxyiodo	$(HO)_2I-$	Fumaroyl (*or* trans-*butenedioyl*)	$-CO-CH=CH-CO-$ (*trans*)
2,3-Dihydroxypropanoyl, *see* Glyceroyl		Furancarbonyl, *see* Furoyl	
3,4-Dimethoxybenzoyl, *see* Veratroyl		Furfuryl (*2- only; preferred to 2-furylmethyl*)	
3,4-Dimethoxyphenethyl	3,4-$(CH_3O)_2C_6H_3CH_2CH-$	Furfurylidene (*2- only*)	
3,4-Dimethoxyphenylacetyl	3,4-$(CH_3O)_2C_6H_3CH_2CO-$	Furoyl (*3- shown; preferred to furancarbonyl*)	
Dimethylamino	$(CH_3)_2N-$		
Dimethylbenzoyl	$(CH_3)_2C_6H_6H_3-CO-$	Furyl	OC_4H_3-
Dioxy	$-O-O-$	3-Furylmethyl	
Diphenylamino	$(C_6H_5)_2N-$		
Diphenylmethylene	$(C_6H_5)_2C=$		
Dithio	$-S-S-$		
Diethiocarboxy	$HSSC-$	Galloyl (*or 3,4,5-trihydroxybenzoyl*)	3,4,5-$(HO)_3C_6H_2-CO-$
Dithiosulfo	HOS_2-		
Dodecanoyl	$CH_3[CH_2]_{10}-CO-$	Geranyl (*from geraniol*)	$C_{10}H_{17}-$
Dodecyl	$CH_3[CH_2]_{11}-$	Glutaminyl	$H_2N-CO-CH_2-CH_2-CH(NH_2)-CO-$
Elaidoyl (*or* trans-9-*octadecenoyl*)	$CH_3[CH_2]_7CH=CH-[CH_2]_7-CO-$	Glutamoyl	$-CO-CH_2-CH_2-CH(NH_2)-CO-$
Epidioxy (as a bridge)	$-O-O-$		
Epidiseleno (as bridge)	$-Se-Se-$	α-Glutamyl	$HOOC[CH_2]_2CH(NH_2)-CO-$
Epidithio (as a bridge)	$-S-S-$		
Epimino (as a bridge)	$-NH-$	γ-Glutamyl	$HOOC-CH(NH_2)-[CH_2]_2-CO-$
Episeleno (as a bridge)	$-Se-$		
Epithio (as a bridge)	$-S-$	Glutaryl (*or pentanedioyl*)	$-CO-[CH_2]_3-CO-$
Epoxy (as a bridge)	$-O-$	Glyceroyl (*or 2,3- dihydroxypropanoyl*)	$HO-CH_2-CH(OH)-CO-$
Ethanesulfonamide	$C_2H_5-SO_2-NH-$		
Ethanoyl, *see* Acetyl		Glycoloyl (*or hydroxyethanoyl*)	$HO-CH_2-CO-$
Ethenyl, *see* Vinyl			
Ethoxalyl	$C_2H_5-OOC-CO-$	Glycyl	H_2N-CH_2-CO-
Ethoxy	C_2H_5-O-	Glycylamino	$H_2N-CH_2-CO-NH-$
Ethoxycarbonyl	$C_2H_5-O-CO-$	Glyoxyloyl	$OHC-CO-$
Ethyl	C_2H_5- or CH_3-CH_2-	Guanidino	$H_2N-C(=NH)-NH-$
Ethylamino	C_2H_5-NH-	Guanyl, *see* Amidino	
Ethylene	$-CH_2-CH_2-$	Heptanamido	$CH_3-[CH_2]_5-CO-NH-$
Ethylenedioxy	$-O-CH_2-CH_2-O-$	Heptanedioyl	$-CO-[CH_2]_5-CO-$
Ethylidene	$CH_3-CH=$	Heptanoyl	$CH_3-[CH_2]_5-CO-$
Ethylidyne	$CH_3-C\equiv$	Heptyl	$CH_3-[CH_2]_5-CH_2-$
Ethylsulfonylamino	$C_2H_5-SO_2-NH-$	Hexadecanoyl	$CH_3-[CH_2]_{14}-CO-$
Ethylthio	C_2H_5-S-	Hexadecyl	$CH_3-[CH_2]_{14}-CH_2-$
Ethynyl	$HC\equiv C-$	Hexamethylene	$-[CH_2]_6-$
Ethynylene	$-C\equiv C-$	Hexanamido	$CH_3-[CH_2]_4-CO-NH-$
Fluoranthenyl	$C_{16}H_9-$	Hexanedioyl (*or adipoyl*)	$-CO-[CH_2]_4-CO-$

TABLE 1.13 Names and Formulas of Organic Radicals (*Continued*)

Name	Formula	Name	Formula
Hexanimidoyl	$CH_3—[CH_2]_4—C(=NH)—$	Iodonio	$^+HI—$
Hexanoyl	$CH_3—[CH_2]_4—CO—$	Iodosyl	$OI—$
Hexanoylamino	$CH_3—[CH_2]_4—CO—NH—$	Iodyl	$O_2I—$
Hexyl	$CH_3—[CH_2]_4—CH_2—$	Isobutoxy (*unsubstituted only*)	$(CH_3)_2CH—CH_2—O—$
Hexylidene	$CH_3—[CH_2]_4—CH=$	Isobutyl (*unsubstituted only*)	$(CH_3)_2CH—CH_2—$
Hexyloxy	$CH_3[CH_2]_5—O—$	Isobutylidene (*unsubstituted only*)	$(CH_3)_2CH—CH=$
Hippuroyl	$C_6H_5—CO—NH—CH_2—CO—$	Isobutylidyne (*unsubstituted only*)	$(CH_3)_2CH—C\equiv$
Histidyl	$N_2C_3H_3—CH_2—CH(NH_2)—CO—$	Isobutyryl (*unsubstituted only; or 2-methylpropanoyl*)	$(CH_3)_2CH—CO—$
Homocysteinyl	$HS—CH_2—CH_2—CH(NH_2)—CO—$	Isocarbonohydrazido	$H_2N—N=C(OH)—NH—NH—$
Homoseryl	$HO—CH_2—CH_2—CH(NH_2)—CO—$	Isocrotonoyl	$CH_3—CH=CH—CO—$ (*cis*)
Hydantoyl	$H_2N—CO—NH—CH_2—CO—$	Isocyanato	$OCN—$
Hydratropoyl (*or 2-phenylpropanoyl*)	$C_6H_5—CH(CH_3)—CO—$	Isocyano	$CN—$
Hydrazi	—NH—NH— (to single atom)	Isohexyl (*unsubstituted only*)	$(CH_3)_2CH—[CH_2]_3—$
Hydrazino	$H_2N—NH—$	Isoleucyl	$C_2H_5—CH(CH_3)—CH(NH_2)—CO$
Hydrazo	—NH—NH— (to different atoms)	Isonicotinoyl (*or 4-pyridinecarbonyl*)	$NC_5H_4—CO—$ (4-)
Hydrazono	$H_2N—N=$	Isopentyl (*unsubstituted only*)	$(CH_3)_2CH—CH_2—CH_2—$
Hydroperoxy	$HO—O—$	Isophthaloyl (*or 1,3-benzenedicarbonyl*)	$—CO—C_6H_4—CO—$ (*m*-)
Hydroseleno	$HSe—$	Isopropenyl (*unsubstituted only; or 1-methylvinyl*)	$CH_2=C(CH_3)—$
Hydroxy	$HO—$	Isopropoxy (*unsubstituted only*)	$(CH_3)_2CH—O—$
Hydroxyamino	$HO—NH—$	Isopropyl (*unsubstituted only*)	$(CH_3)_2CH—$
o-Hydroxybenzoyl (*or salicyloyl*)	*o*-$HO—C_6H_4—CO—$	*p*-Isopropylbenzoyl	*p*-$(CH_3)_2CH—C_6H_4—CO—$
m-Hydroxybenzoyl	*m*-$HO—C_6H_4—CO—$	Isopropylbenzyl	$(CH_3)_2CH—C_6H_4—CH_2—$
p-Hydroxybenzoyl	*p*-$HO—C_6H_4—CO—$	Isopropylidene	$(CH_3)_2C=$
Hydroxybutanedioyl, *see* Maloyl		Isoselenocyanato	$SeCN—$
2-Hydroxy-2,2-diphenyl ethanoyl, *see* Benziloyl		Isosemicarbazido	$H_2N—NH—C(OH)=N—$
Hydroxyethanoyl, *see* Glycoloyl		Isothiocyanato	$SCN—$
Hydroxyimino	$HO—N=$	Isothioureido	$HN=C(SH)—NH—$, $H_2N—C(SH)=N—$
4-Hydroxy-3-methoxybenzoyl (*or vanilloyl*)	4-HO,3-$CH_3O—C_6H_3—CO—$	Isoureido	$HN=C(OH)—NH—$, $H_2N—C(OH)=N—$
3-Hydroxy-2-phenylpropanoyl (*or tropoyl*)	$C_6H_5—CH(CH_2OH)—CO—$	Isovaleryl (*unsubstituted only; or 3-methylbutanoyl*)	$(CH_3)_2CH—CH_2—CO—$
Hydroxypropanedioyl (*or tartronoyl*)	$—CO—CH(OH)—CO—$	Lactoyl	$CH_3—CH(OH)—CO—$
2-Hydroxypropanoyl (*or lactoyl*)	$CH_3—CH(OH)—CO—$	Lauroyl (*unsubstituted only*)	$CH_3—[CH_2]_{10}—CO—$
Icosyl	$CH_3—[CH_2]_{18}—CH_2—$		
Imino	$—NH—$, $HN=$		
Iminomethylamino	$HN=CH—NH—$		
Iodo	$I—$		
Iodoformyl	$I—CO—$		

TABLE 1.13 Names and Formulas of Organic Radicals (*Continued*)

Name	Formula
Leucyl	$(CH_3)_2CH—CH_2—CH(NH_2)—CO—$
Lysyl	$H_2N—[CH_2]_4—CH(NH_2)—CO—$
Maleoyl	$—CO—CH=CH—CO—$
Malonyl	$—CO—CH_2—CO—$
Maloyl	$—CO—CH(OH)—CH_2—CO—$
Mercapto-	$HS—$
Mesaconoyl (*unsubstituted only*)	$—CO—C(CH_3)=CH—CO—$
Mesityl	$2,4,6\text{-}(CH_3)_3C_6H_2—$
Mesoxalo	$HOOC—CO—CO—$
Mesoxalyl	$—CO—CO—CO—$
Mesyl	$CH_3—SO_2—$
Methacryloyl (*or 2-methylpropenoyl*)	$CH_2=C(CH_3)—CO—$
Methaneazo	$CH_3—N=N—$
Methaneazoxy	$CH_3—N_2O—$
Methanesulfinamido	$CH_3—SO—NH—$
Methanesulfinyl	$CH_3—SO—$
Methanesulfonamido	$CH_3—SO_2—NH—$
Methanesulfonyl, *see* Mesyl	
Methanoyl, *see* Formyl	
Methionyl	$CH_3—S—CH_2—CH_2—CH(NH_2)—CO—$
Methoxalyl	$CH_3OOC—CO—$
Methoxy	$CH_3O—$
Methoxybenzoyl (*o-*, *m-*, *or p-*)	$CH_3O—C_6H_4—CO—$
Methoxycarbonyl	$CH_3O—CO—$
Methoxyimino	$CH_3O—N=$
Methoxyphenyl	$CH_3O—C_6H_4—$
Methoxysulfinyl	$CH_3O—SO—$
Methoxysulfonyl	$CH_3O—SO_2—$
Methoxy(thiosulfonyl)	$CH_3O—S_2O—$
Methyl	$CH_3—$
Methylallyl	$CH_2=C(CH_3)—CH_2—$
Methylamino	$CH_3—NH—$
Methylazo	$CH_3—N=N—$
Methylazoxy	$CH_3—N_2O—$
α-Methylbenzyl	$C_6H_5—CH(CH_3)—$
Methylbenzyl	$CH_3—C_6H_4—CH_2—$
3-Methylbutanoyl	$(CH_3)_2CH—CH_2—CO—$
cis-Methylbutenedioyl	$CH_3—C(=CH—CO—)—CO—$
trans-Methylbutenedioyl	$—CO—CH=C(—CH_3)—CO—$
Methyldithio	$CH_3—S—S—$
Methylene	$—CH_2—$, $H_2C=$
Methylenedioxy	$—O—CH_2—O—$
3,4-Methylenedioxybenzoyl	$3,4\text{-}CH_2O_2:C_6H_3—CO—$

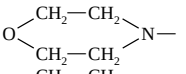
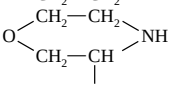
Name	Formula
5-Methylhexyl	$(CH_3)_2CH—[CH_2]_4—$
Methylidyne	$HC\equiv$
Methylsulfinimidoyl	$CH_3—S(=NH)—$
Methylsulfinohydrazonoyl	$CH_3—S(=NNH_2)—$
Methylsulfinohydroximoyl	$CH_3—S(=N—OH)—$
Methylsulfinyl	$CH_3—SO—$
Methylsulfinylamino	$CH_3—SO—NH—$
Methylsulfonohydrazonoyl	$CH_3—S(O)(NNH_2)—$
Methylsulfonimidoyl	$CH_3—S(O)(=NH)—$
Methylsulfonohydroxamoyl	$CH_3—S(O)(N—OH)—$
Methylsulfonyl	$CH_3—SO_2—$
Methylthio	$CH_3S—$
(Methylthio)sulfonyl	$CH_3S—SO_2—$
1-Methylvinyl, *see* Isopropenyl	
Morpholino (*4- only*)	
Morpholinyl (*3- shown*)	
Myristoyl (*unsubstituted only*)	$CH_3—[CH_2]_{12}—CO—$
Naphthalenazo	$C_{10}H_7—N=N—$
Naphthalenecarbonyl, *see* Naphthoyl	
Naphthoyl	$C_{10}H_7—CO—$
Naphthoyloxy	$C_{10}H_7—CO—O—$
Naphthyl	$C_{10}H_7—$
Naphthylazo	$C_{10}H_7—N=N—$
Naphthylene	$—C_{10}H_6—$
Naphthylenebisazo	$—N=N—C_{10}H_6—N=N—$
Naphthyloxy	$C_{10}H_7—O—$
Neopentyl (*unsubstituted only*)	$(CH_3)_3C—CH_2—$
Nicotinoyl	$NC_5H_4—CO—$ (3-)
Nitrilo	$N\equiv$
Nitro	$O_2N—$
aci-Nitro	$HO—(O=)N=$
Nitroso	$ON—$
Nonanedioyl	$—CO—[CH_2]_7—CO—$
Nonanoyl	$CH_3—[CH_2]_7—CO—$
Nonyl	$CH_3—[CH_2]_7—CH_2—$
Norbornyl	$C_7H_{11}—$
Norbornylyl, *see* Norbornyl	
Norcamphyl, *see* Norbornyl	
Norleucyl	$CH_3—[CH_2]_3—CH(NH_2)—CO—$
Norvalyl	$CH_3—CH_2—CH_2—CH(NH_2)—CO—$
Octadecanoyl	$CH_3—[CH_2]_{16}—CO—$

TABLE 1.13 Names and Formulas of Organic Radicals (*Continued*)

Name	Formula	Name	Formula
cis-9-Octadecenoyl	$H[CH_2]_8—CH═CH—[CH_2]_7—CO—$	Phenylsulfamoyl	$C_6H_5—NH—SO_2$
		Phenylsulfinyl	$C_6H_5—SO—$
Octadecyl	$CH_3—[CH_2]_{16}—CH_2—$	Phenylsulfonyl	$C_6H_5—SO_2—$
Octanedioyl	$—CO—[CH_2]_6—CO—$	Phenylsulfonylamino	$C_6H_5—SO_2—NH—$
Octanoyl	$CH_3—[CH_2]_6—CO—$	Phenylthio	$C_6H_5—S—$
Octyl	$CH_3—[CH_2]_6—CH_2—$	3-Phenylureido	$C_6H_5—NH—CO—NH—$
Oleoyl	$H[CH_2]_8—CH═CH—[CH_2]_7—CO—$	Phthalamoyl	$H_2N—CO—C_6H_4—CO—$ (*o*-)
Ornithyl	$H_2N—[CH_2]_3—CH(NH_2)—CO—$	Phthalidyl	$C_6H_4—CO—O—CH—$
Oxalacetyl	$—CO—CH_2—CO—CO—$	Phthalimido	$CO—C_6H_4—CO—N—$
		Phthaloyl	$—CO—C_6H_4—CO—$ (*o*-)
Oxalaceto	$HOOC—CO—CH_2—CO—$	Picryl	$2,4,6\text{-}(NO_2)_3C_6H_2—$
		Pimeloyl (*unsubstituted only*)	$—CO—[CH_2]_5—CO—$
Oxalo	$HOOC—CO—$		
Oxalyl	$—CO—CO—$	Piperidino (*1- only*)	$C_5H_{10}N—$
Oxamoyl	$H_2N—CO—CO—$	Piperidyl (*2-*, *3-*, *4-*)	$NC_5H_{10}—$
Oxido	$^{-}O—$ (ion)	Piperonyl	$3,4\text{-}CH_2O_2:C_6H_3—CH_2—$
Oxo	$O═$	Pivaloyl (*unsubstituted only*)	$(CH_3)_3C—CO—$
Oxonio	$^{+}H_2O—$		
Oxy	$—O—$	Polythio	$—S_4—$
Palmitoyl (*unsubstituted only*)	$CH_3—[CH_2]_{14}—CO—$	Propanedioyl, *see* Malonyl	
Pentafluorothio	$F_5S—$	Propanoyl, *see* Propionyl	
Pentamethylene	$—CH_2—CH_2—CH_2—CH_2—CH_2—$	Propargyl, *see* 2-Propynyl	
Pentanedioyl, *see* Glutaryl		Propenoyl, *see* Acryloyl	
		1-Propenyl	$CH_3—CH═CH—$
Pentanoyl, *see* Valeryl		2-Propenyl, *see* Allyl	
Pentenyl (*2- shown*)	$CH_3—CH_2—CH═CH—CH_2—$	Propenylene	$—CH_2—CH═CH—$
		Propioloyl	$CH≡C—CO—$
Pentyl	$CH_3—CH_2—CH_2—CH_2—CH_2—$	Propionamido	$CH_3—CH_2—CO—NH—$
		Propionyl	$CH_3—CH_2—CO—$
Pentyloxy	$CH_3—[CH_2]_4—O—$	Propionylamino	$CH_3—CH_2—CO—NH—$
Perchloryl	$O_3Cl—$	Propionyloxy	$CH_3—CH_2—CO—O—$
Phenacyl	$C_6H_5—CO—CH_2—$	Propoxy	$CH_3—CH_2—CH_2—O$
Phenacylidene	$C_6H_5—CO—CH═$	Propyl	$CH_3—CH_2—CH_2—$
Phenanthryl	$C_{14}H_9—$	Propylene	$—CH(CH_3)—CH_2—$
Phenethyl	$C_6H_5—CH_2—CH_2—$	Propylidene	$CH_3—CH_2—CH═$
Phenetidino (*o-*, *m-*, *or p-*)	$C_2H_5O—C_6H_4—NH—$	Propylidyne	$CH_3—CH_2—C≡$
Phenoxy	$C_6H_5—O—$	Propynoyl, *see* Propiolyl	
Phenyl	$C_6H_5—$	1-Propynyl	$CH_3—C≡C—$
Phenylacetyl	$C_6H_5—CH_2—CO—$	2-Propynyl	$HC≡C—CH_2—$
Phenylazo	$C_6H_5—N═N—$	Protocatechuoyl	$3,4\text{-}(HO)_2C_6H_3—CO—$
Phenylazoxy	$C_6H_5—N_2O—$	3-Pyridinecarbonyl	$NC_5H_4—CO—$ (3-)
Phenylcarbamoyl	$C_6H_5—NH—CO$	4-Pyridinecarbonyl	$NC_5H_4—CO—$ (4-)
Phenylene	$—C_6H_4—$	Pyridinio	$^{+}NC_5H_5—$ (ion)
Phenylenebisazo	$—N═N—C_6H_4—N═N—$	Pyridyl	$NC_5H_4—$
		2-Pyridylcarbonyl	$NC_5H_4—CO—$ (2-)
Phenylimino	$C_6H_5—N═$	Pyridyloxy	$NC_5H_4—O—$
2-Phenylpropanoyl	$C_6H_5—CH(CH_3)—CO—$	Pyruvoyl	$CH_3—CO—CO—$
3-Phenylpropenoyl, *see* Cinnamoyl		Salicyl	$o\text{-}HO—C_6H_4—CH_2—$
		Salicylidene	$o\text{-}HO—C_6H_4—CH═$
3-Phenylpropyl	$C_6H_5—CH_2—CH_2—CH_2—$	Salicyloyl	$o\text{-}HO—C_6H_4—CO—$
		Sarcosyl	$CH_3—NH—CH_2—CO—$

TABLE 1.13 Names and Formulas of Organic Radicals (*Continued*)

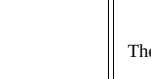
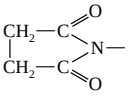
Name	Formula	Name	Formula
Sebacoyl (*unsubstituted only*)	—CO—$[CH_2]_8$—CO—	(Terthiophen)yl	SC_4H_3—SC_4H_2—SC_4H_2—
		Tetradecanoyl	CH_3—$[CH_2]_{12}$—CO—
Seleneno	HOSe—	Tetradecyl	CH_3—$[CH_2]_{12}$—CH_2—
Selenino	HO_2Se—	Tetramethylene	—CH_2—CH_2—CH_2—CH_2—
Seleninyl	OSe═		
Seleno	—Se—		
Selenocyanato	NC—Se—	Thenoyl (*2- shown*)	
Selenoformyl	HSeC—		
Selenonio	^+H_2Se— (ion)	Thenyl	SC_4H_3—CH_2—
Selenono	HO_3Se—	Thienyl	SC_4H_3—
Selenonyl	O_2Se—	Thio	—S—
Seleneureido	H_2N—CSe—NH—	Thioacetyl	CH_3—CS—
Selenoxo	(C)═Se	Thiobenzoyl	C_6H_5—CS—
Semicarbazido	H_2N—CO—NH—NH—	Thiocarbamoyl	H_2N—CS—
Semicarbazono	H_2N—CO—NH—N═	Thiocarbazono	HN═N—CS—NH—NH—
Seryl	HO—CH_2—$CH(NH_2)$—CO—	Thiocarbodiazono	HN═N—CS—N═N—
Stearoyl (*unsubstituted only*)	CH_3—$[CH_2]_{16}$—CO—	Thiocarbonohydrazido	H_2N—NH—CS—NH—NH—
Styryl	C_6H_5—CH═CH—	Thiocarbonyl	—CS—, SC═
Suberoyl (*unsubstituted only*)	—CO—$[CH_2]_6$—CO—	Thiocarboxy	HSOC—, HS—CO—
		Thiocyanato	NCS—
Succinamoyl	H_2N—CO—CH_2—CH_2—CO—	Thioformyl	SHC—, HCS—
		Thiophenecarbonyl, *see* Thenoyl	
Succinimido		Thiosemicarbazido	H_2N—CS—NH—NH—
		Thiosulfino	HOS_2—
		Thiosulfo	HO_2S_2—
Succinimidoyl	—C(═NH)—CH_2—CH_2C(═NH)—	Thioreido	H_2N—CS—NH—
		Thioxo	S═
Succinyl	—CO—CH_2—CH_2—CO—	Threonyl	CH_3—CH(OH)—$CH(NH_2)$—CO—
Sulfamoyl	H_2N—SO_2—		
Sulfanilamido	*p*-H_2N—C_6H_4—SO_2—NH—	Toluenesulfonyl (*o-, m-*)	CH_3—C_6H_4—SO_2—
		Toluidino (*o-, m-, or p-*)	CH_3—C_6H_4—NH—
Sulfanilyl	*p*-H_2N—C_6H_4—SO_2—	Toluoyl (*o-, m-, or p-*)	CH_3—C_6H_4—CO—
Sulfenamoyl	H_2N—S—	Tolyl (*o-, m-, or p-*)	CH_3—C_6H_4—
Sulfeno	HO—S—	Tolylsulfonyl	CH_3—C_6H_4—SO_2—
Sulfido	$^-$S— (ion)	Tosyl (*p- only*)	*p*-CH_3—C_6H_4—SO_2—
Sulfinamoyl	H_2N—SO—	Triazano	H_2N—NH—NH—
Sulfino	HO_2S—	Triazeno	H_2N—N═N—
Sulfinyl	—SO—	Trichlorothio	Cl_3S—
Sulfo	HO—SO_2—	Tridecanoyl	CH_3—$[CH_2]_{11}$—CO—
Sulfoamino	HO_2S—NH—	Tridecyl	CH_3—$[CH_2]_{12}$—
Sulfonato	^-O_3S— (ion)	Trifluorothio	F_3S—
Sulfonio	^+H_2S— (ion)	3,4,5-Trihydroxybenzoyl	3,4,5-$(HO)_3C_6H_2$—CO—
Sulfonyl	—SO_2—	Trimethylammonio	$(CH_3)_3N^+$— (ion)
Sulfonyldioxy	—O—SO_2—O—	Trimethylanilino (*all isomers*)	$(CH_3)_3C_6H_2$—NH—
Tartaroyl	—CO—CH(OH)—CH(OH)—CO—	Trimethylene	—CH_2—CH_2—CH_2—
Tartronoyl	—CO—CH(OH)—CO—	Trimethylenedioxy	—O—CH_2—CH_2—CH_2—O—
Tauryl	H_2N—CH_2—CH_2—SO_2—		
Telluro	Te replacing O	Triphenylmethyl	$(C_6H_5)_3C$—
Terephthaloyl	—CO—C_6H_4—CO— (*p-*)	Trithio	—S_3—
Terphenylyl	C_6H_5—C_6H_4—C_6H_4—	Trithiosulfo	HS—S_3—

TABLE 1.13 Names and Formulas of Organic Radicals (*Continued*)

Name	Formula	Name	Formula
Trityl	$(C_6H_5)_3C$—	Vanilloyl	3,4-$CH_3O(HO)C_6H_3$—CO—
Tropoyl	C_6H_5—$CH(CH_2OH)$—CO—	Vanillyl	3,4-$CH_3O(HO)C_6H_3$—CH_2—
Tyrosyl	*p*-HO—C_6H_4—CH_2—$CH(NH_2)$—CO—	Veratroyl	3,4-$(CH_3O)_2C_6H_3$—CO—
Undecanoyl	CH_3—$[CH_2]_9$—CO—	Veratryl	3,4-$(CH_3O)_2C_6H_2$—CH_2—
Undecyl	CH_3—$[CH_2]_9$—CH_2—		
Ureido	H_2N—CO—NH—		
Ureylene	—NH—CO—NH—	Vinyl	CH_2═CH—
Valeryl	CH_3—$[CH_2]_3$—CO—	Vinylene	—CH═CH—
Valyl	$(CH_3)_2CH$—$CH(NH_2)$—CO—	Xylidino (*all isomers*)	$(CH_3)_2C_6H_3$—NH—
		Xylyl (*all isomers*)	$(CH_3)_2C_6H_3$—

1.2 PHYSICAL PROPERTIES OF PURE SUBSTANCES

TABLE 1.14 Empirical Formula Index of Organic Compounds

The alphanumeric designations are keyed to Table 1.15.

Br_2OS: t149
$ClHO_3S$: c248
ClH_4NO: h139
Cl_2OS: t150
Cl_2H_2Si: d270a
Cl_3HSi: t249
Cl_3PS: t158
H_3NO_3S: s23
H_4N_2: h85
H_6Si_2: d791

C_1

CBr_4: c13
$CBrClF_2$: b301
$CBrCl_3$: b432
$CBrF_3$: b434
CBrN: c325
CBr_2F_2: d93
CBr_4: c13
$CClF_3$: c264
$CClNO_3S$: c249
CCl_2F_2: d218
CCl_3D: c146
CCl_3F: t237
CCl_4: c14
CCl_4S: t240
CD_2Cl_2: d236
CD_4O: m36
CD_7O: m40
$CFCl_3$: f30
CF_4: c15
$CHBrCl_2$: b316
$CHBr_2Cl$: d88
$CHBr_2F$: d104a
$CHBr_3$: t204
$CHClF_2$: c101
$CHCl_2F$: d233
$CHCl_3$: c145
CHF_3: t307
CHF_3O_3S: t308
CHI_3: i33
CH_2BrCl: b305
CH_2Br_2: d110
CH_2Cl_2: d235
CH_2F_2: d409
CH_2I_2: d452
CH_2N_2: c318, d63
CH_2N_4: t131
CH_2O: f32
$(CH_2O)_x$: p1
CH_2O_2: f36
CH_2O_3: g29
CH_2S_3: t451
CH_3Br: b354
CH_3Br_3Ge: m260
CH_3Cl: c157
CH_3ClO_2S: m36
CH_3Cl_3Si: m450, t242
CH_3DO: m39
CH_3F: f18
CH_3I: i37
CH_3NO: f33
CH_3NO_2: m325, n56
CH_3NO_3: m324
CH_3N_5: a294
CH_4: m33
CH_4Cl_2Si: d240
CH_4N_2O: f38, u16
CH_4N_2S: t161
$CH_4N_4O_2$: n54
CH_4O: m38
$^{13}CH_4O$: m41
CH_4O_2: m279
CH_4O_3S: m34
CH_4S: m37
CH_5AsO_3: m137
CH_5N: m127
CH_5NO_3S: a201
CH_5N_3: g30
CH_5N_3S: t160
CH_6ClN_3O: s3
CH_6N_2: m274
CH_6N_4: a180
CH_6N_4O: c9
CI_4: c16
CN_4O_8: t123
CS_2: c10
CO: c11
COS: c12

C_2

$C_2Br_2ClF_3$: d90
$C_2Br_2Cl_4$: d129
$C_2Br_2F_4$: d130
$C_2Br_2O_2$: o54
C_2ClF_3: c263
$C_2Cl_2F_4$: d270b, d271
$C_2Cl_2O_2$: o55
$C_2Cl_3F_3$: t256, t257
C_2Cl_3N: t222

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

C_2Cl_4: t38
$C_2Cl_4F_2$: d411, d412, t36
C_2Cl_4O: t224
C_2Cl_6: h27
C_2D_3N: a30
$C_2D_4O_2$: a21
C_2D_6OS: d698
C_2F_4: t65
C_2F_6: h42
$C_2F_6O_5S_2$: t309
$C_2HBrClF_3$: b308
$C_2HBr_2F_3$: d133
C_2HBr_2N: d77
C_2HBr_3: t203
C_2HBr_3O: t199
$C_2HBr_3O_2$: t200
C_2HClF_2: c100a
$C_2HClF_2O_2$: c98
C_2HCl_3: t235
C_2HCl_3O: d186, t218
$C_2HCl_3O_2$: t219
C_2HCl_5: p7
$C_2HF_3O_2$: t300
C_2H_2: a41
C_2H_2BrClO: b255
$C_2H_2Br_2$: d99, d100
$C_2H_2Br_2F_2$: d92
$C_2H_2Br_2O$: b254
$C_2H_2Br_2O_2$: d76
$C_2H_2Br_4$: t16
$C_2H_2ClF_3$: c262
C_2H_2ClN: c30
$C_2H_2Cl_2$: d227, d228, d229
$C_2H_2Cl_2O$: c34
$C_2H_2Cl_2O_2$: d182
$C_2H_2Cl_3NO$: t217
$C_2H_2Cl_4$: t36a, t37
$C_2H_2F_2$: d408
$C_2H_2F_3NO$: t299
$C_2H_2F_4$: t64
$C_2H_2N_2S_3$: d488
C_2H_2O: k1
$C_2H_2O_2$: g28
$C_2H_2O_3$: g29
$C_2H_2O_4$: o52, o53
C_2H_3Br: b336
C_2H_3BrO: a35
$C_2H_3BrO_2$: b249
$C_2H_3Br_2Cl_3Si$: d101
$C_2H_3Br_3O$: t202
C_2H_3Cl: c129
$C_2H_3ClF_2$: c100
C_2H_3ClO: a37, c23a
$C_2H_3ClO_2$: c27, m194
$C_2H_3Cl_3$: t231, t232
$C_2H_3Cl_3O$: t233
$C_2H_3Cl_3Si$: t258
$C_2H_3DO_2$: a20
C_2H_3FO: a43
$C_2H_3FO_2$: f5
$C_2H_3F_3O$: t305
$C_2H_3F_3O_3S$: m453
C_2H_3IO: a48
$C_2H_3IO_2$: i21
C_2H_3N: a29
C_2H_3NO: m288
C_2H_3NS: m294, m440
$C_2H_3N_3$: t197
$C_2H_3N_3S_2$: a284
C_2H_4: e131
C_2H_4BrCl: b303
C_2H_4BrNO: b247
$C_2H_4Br_2$: d96, d97
C_2H_4ClNO: c24
C_2H_4ClO: b165a
$C_2H_4Cl_2$: d225, d226
$C_2H_4Cl_2O$: d237
$C_2H_4Cl_6Si_2$: b227
$C_2H_4F_2$: d407
C_2H_4INO: i20
$C_2H_4I_2$: d451
$C_2H_4N_2$: a109
$C_2H_4N_2O_2$: o58
$C_2H_4N_2S_2$: d795
$C_2H_4N_4$: a289, d281
$C_2H_4N_4O_2$: a314
C_2H_4O: e147
C_2H_4OS: t147
$C_2H_4O_2$: a19, h87, m257
$C_2H_4O_2S$: m16
$C_2H_4O_3$: h88, p60
$C_2H_4O_5S$: s26
C_2H_4S: e148
$C_2H_5AlCl_2$: e61
C_2H_5Br: b329
$C_2H_5BrNaO_2S$: b330
C_2H_5BrO: b331, b369
C_2H_5Cl: c121
C_2H_5ClHg: e198
C_2H_5ClO: c122, c156, c173
C_2H_5ClS: c174
$C_2H_5Cl_2OPS$: e124
$C_2H_5Cl_2O_2P$: e123
$C_2H_5Cl_3Si$: c171, e269, t236
C_2H_5DO: e28
C_2H_5F: f17
C_2H_5I: i31
C_2H_5IO: i32
C_2H_5N: e146
C_2H_5NO: a5, a6, m255, m291
$C_2H_5NO_2$: e225, g26, m187, n52
$C_2H_5NO_3$: e224
C_2H_5NS: t138
$C_2H_5N_3O_2$: b238, o57
C_2H_6: e20
C_2H_6AlCl: d533
C_2H_6BrN: b333
C_2H_6Cd: d578
C_2H_6ClN: c126
$C_2H_6ClNO_2S$: d692
$C_2H_6ClO_2PS$: d582
$C_2H_6Cl_2Si$: d222
C_2H_6Hg: d631
$C_2H_6N_2$: a8
$C_2H_6N_2O$: m460, n78
$C_2H_6N_2O_2$: m275
$C_2H_6N_2S$: m444
$C_2H_6N_4O$: o56
C_2H_6O: d603, e27
C_2H_6OS: d697, m20
$C_2H_6O_2$: e21a, e135
$C_2H_6O_2S$: d696
$C_2H_6O_3S$: d695, e25, m301
$C_2H_6O_4S$: d693
$C_2H_6O_5S_2$: m35
C_2H_6S: d694, e26a
$C_2H_6S_2$: d600, e24
C_2H_6Te: d700
C_2H_6Zn: d709
$C_2H_7AsO_2$: d560
C_2H_7ClSi: c111
C_2H_7N: d534, e63
C_2H_7NO: a162, a163, e29
$C_2H_7NO_3S$: a160
$C_2H_7NO_4S$: a169
C_2H_7NS: a161
$C_2H_7N_5$: b137
$C_2H_7O_3P$: d625
$C_2H_8N_2$: d623, d624, e21, e133
$C_2H_8N_2O$: h125
C_2H_9BD: b243
$C_2H_{10}BN$: b242

C_3

$C_3Br_2F_5$: d105
$C_3Cl_3N_3$: t255
$C_3Cl_3N_3O_3$: t239
C_3Cl_6: h30
C_3Cl_6O: a27, h2
C_3F_6: h44
C_3HCl_5O: p5
C_3H_2ClN: c35
$C_3H_2Cl_2O_2$: m6

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

C_4

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

$C_4H_2O_4$: q42
C_4H_3IS: i52
$C_4H_3N_3O_4$: n88
C_4H_4: b489
$C_4H_4BrNO_2$: b422
$C_4H_4Br_2O_2$: d86
$C_4H_4Br_2O_4$: d128
$C_4H_4ClNO_2$: c247
$C_4H_4ClO_3$: c28
$C_4H_4Cl_2$: d213
$C_4H_4Cl_2O_2$: s19
$C_4H_4Cl_2O_3$: c25
$C_4H_4N_2$: b456, p251, p256, p277, s18
$C_4H_4N_2O_2$: d448, p278
$C_4H_4N_2O_2S$: d437
$C_4H_4N_2O_3$: b1
$C_4H_4N_2O_5$: a73
$C_4H_4N_4$: d50
C_4H_4O: f45
$C_4H_4O_2$: d483
$C_4H_4O_3$: s16
$C_4H_4O_4$: f42, m1
C_4H_4S: t151
$C_4H_5BrO_2$: b283
$C_4H_5BrO_4$: b421
C_4H_5Cl: c74, c74a, c83
$C_4H_5ClN_2O_2$: c184
C_4H_5ClO: c310, c408, m31
$C_4H_5ClO_2$: a82
$C_4H_5ClO_3$: c194, e232
$C_4H_5Cl_3O_2$: e268
C_4H_5N: b482, c309, c407, m30a, p279
C_4H_5NO: m47, m295
$C_4H_5NO_2$: m201, s17
$C_4H_5NO_2S$: e39
$C_4H_5NO_3$: h183
C_4H_5NS: a88, m432
$C_4H_5N_3$: a278, i8
$C_4H_5N_3O$: a194
$C_4H_5N_3OS$: a187
$C_4H_5N_3O_2$: a152, a153, c322, m338
$C_4H_5N_4O$: d49
C_4H_6: b448, b449, b610a, b610b
$C_4H_6Br_2O$: b374
$C_4H_6Br_2N_2O_2$: d95
$C_4H_6Br_2O_2$: d87
C_4H_6ClN: c86
$C_4H_6Cl_2$: c89, d211, d212
$C_4H_6Cl_2O$: c87
$C_4H_6Cl_2O_2$: m229
$C_4H_6Cl_3NSi$: t250
$C_4H_6N_2$: a149, m284, m285, m286
$C_4H_6N_2O_2$: e121, m273
$C_4H_6N_2S$: a225
$C_4H_6N_2S_2$: d584
$C_4H_6N_4O$: d39
$C_4H_6N_4O_3$: a71
C_4H_6O: b488, c306, d421, m27, m407
$C_4H_6O_2$: b466, b483, b484, b485, b611, b616, b617, c307, c409, m29, m126, v5
$C_4H_6O_2S$: b450
$C_4H_6O_3$: a22, a24, m355, o60, p230
$C_4H_6O_4$: d652, s15
$C_4H_6O_4S$: m25, t143
$C_4H_6O_5$: d690, h186, h187, o67
$C_4H_6O_6$: t1, t2, t3, t4
C_4H_7Br: b276, b277, b278
$C_4H_7BrO_2$: b282, b332, b368, b373, e83, m156
C_4H_7Cl: c79, c80, c81, c181, c182, c312
C_4H_7ClO: b620, c78, c136, i85
$C_4H_7ClO_2$: c84, c85, e105, m196, p228
$C_4H_7Cl_3O$: t241
$C_4H_7FO_2$: e153
C_4H_7N: b618, i83
C_4H_7NO: h153, i115, m28, m99a, m352, p236, p285
$C_4H_7NO_2$: b467, h146, m351
$C_4H_7NO_3$: a46, e233, s13
$C_4H_7NO_4$: a304, i7
C_4H_7NS: m434
$C_4H_7N_3O$: c302
C_4H_8: b477, b478, b479, c333, m399
C_4H_8BrCl: b298, b306
$C_4H_8Br_2$: d81, d82, d83, d84
$C_4H_8Br_2O$: b148
$C_4H_8Br_2O_2$: d85
$C_4H_8Cl_2$: d210
$C_4H_8Cl_2O$: b163, d230
$C_4H_8I_2$: d450
$C_4H_8N_2$: d535
$C_4H_8N_2O$: a102
$C_4H_8N_2O_2$: d610, s14
$C_4H_8N_2O_3$: a313, g27
$C_4H_8N_2S$: a97, t85
C_4H_8O: b475, b486, b487, b612, c311, e3, e276, i79, m106, m389, m400, t69
$C_4H_8O_2$: b480, b481, b614, d732, d733, e57, h107, h108, i81. m64, m401, p234
$C_4H_8O_2S$: e196, m299, t107
$C_4H_8O_3$: e24, e153, h120, h138, m70, m296, m302
C_4H_8S: a90, t87
$C_4H_8S_2$: d792
C_4H_9Br: b274, b275, b371, b372
C_4H_9BrO: b337
$C_4H_9BrO_2$: b319
C_4H_9Cl: c75, c76, c179, c180
C_4H_9ClO: a64, c77, c131, m74
$C_4H_9ClO_2$: c105, c123, m67
C_4H_9ClSi: c112
$C_4H_9Cl_3Si$: b604, b603, d215
$C_4H_9Cl_3Sn$: b600
C_4H_9F: f21
C_4H_9I: i26, i27, i38, i39
C_4H_9N: e53, p280
C_4H_9NO: a311, b476, b613, d526, i80, m110, m463
$C_4H_9NO_2$: a133, a133a, a134, b578, b579, h119, i73, n48
$C_4H_9NO_2S$: a200
$C_4H_9NO_3$: a185, a186, i72, m341, n49
$C_4H_9NO_5$: t442
C_4H_9NSi: c331
$C_4H_9N_3O_2$: c301
C_4H_{10}: b454, m390
$C_4H_{10}AlCl$: d320, e62
$C_4H_{10}ClO_2PS$: d351
$C_4H_{10}ClO_3P$: d350
$C_4H_{10}Cl_2Si$: b165
$C_4H_{10}Cl_4Si_2$: b174
$C_4H_{10}N_2$: p178
$C_4H_{10}N_2O$: a227
$C_4H_{10}N_2O_4S$: a8
$C_4H_{10}O$: b473, b474, d365, m397, m398, m404
$C_4H_{10}OS$: e180
$C_4H_{10}OS_2$: b208
$C_4H_{10}O_2$: b457, b457a, b457b, b458, b563, d504, d505, e40, e141, m105, m393
$C_4H_{10}O_2S$: t144
$C_4H_{10}O_2S_2$: d484, h123
$C_4H_{10}O_3$: b198, b472, d361, o62, t378
$C_4H_{10}O_3S$: d399
$C_4H_{10}O_4$: e19
$C_4H_{10}O_4S$: d397

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

$C_4H_{10}S$: b470, b471, d398, i104, m394, m395, m396, m406
$C_4H_{10}S_2$: b468, d356
$C_4H_{10}S_3$: b209
$C_4H_{10}Zn$: d405
$C_4H_{11}ClSi$: c183
$C_4H_{11}N$: b453, b509, b510, b511, d323, d604, i66, m293
$C_4H_{11}NO$: a135, a164, a203, a216, d376, d539, e44, e67, m112
$C_4H_{11}NO_2$: a215, d297, d506
$C_4H_{11}NO_3$: t439
$C_4H_{11}OP$: d390
$C_4H_{11}O_2PS_2$: d358
$C_4H_{11}O_3P$: d375
$C_4H_{12}BrN$: t93
$C_4H_{12}ClN$: d324, t94
$C_4H_{12}Ge$: t109
$C_4H_{12}IN$: t95
$C_4H_{12}N_2$: b455, b560, b562, d41, d605, m391, m392
$C_4H_{12}N_2O$: a165
$C_4H_{12}N_2S_4$: b183
$C_4H_{12}OSi$: m119
$C_4H_{12}O_2Si$: d502
$C_4H_{12}O_3Si$: m455
$C_4H_{12}Pb$: t112
$C_4H_{12}Si$: t118
$C_4H_{12}Sn$: t121
$C_4H_{13}N_3$: d362
$C_4H_{14}BN$: b239
$C_4H_{14}OSi_2$: t106
$C_4H_{16}O_4Si_4$: t104

C_5

C_5Cl_5N: p10
C_5Cl_6: h25
C_5D_5N: p258
C_5H_3BrS: b426, b427
$C_5H_3Br_2N$: d127
C_5H_3ClOS: t153
$C_5H_3ClO_2$: f55
C_5H_3ClS: c251
$C_5H_3Cl_2N$: d268, d269
$C_5H_3N_3$: p252
C_5H_4BrN: b416, b417
C_5H_4ClN: c242
C_5H_4FN: f26
$C_5H_4F_8O$: o20
$C_5H_4N_2O_2$: p253
$C_5H_4N_2O_3$: n76
$C_5H_4N_4O_3$: u17
C_5H_4OS: t154
$C_5H_4O_2$: f44
$C_5H_4O_2S$: t155
$C_5H_4O_3$: c285, f54
$C_5H_5ClN_2$: a148
$C_5H_5ClN_2O_2$: c168
C_5H_5N: p257
C_5H_5NO: h179, h180, h181, p271
$C_5H_5NO_2$: d448, h183
$C_5H_5N_3O_2$: a243
$C_5H_5N_3O_4$: a158
$C_5H_5N_5$: a61
C_5H_6: c395, m174
$C_5H_6BrClN_2O_2$: b302
$C_5H_6Br_2N_2O_2$: d76
$C_5H_6Cl_2NO_2$: d220
$C_5H_6Cl_2O_2$: g18
$C_5H_6N_2$: a275, a276, a277, g17, m408, v12
$C_5H_6N_2O$: a47, a193
$C_5H_6N_2OS$: h140, h141
C_5H_6O: m259
C_5H_6OS: f48, m443
$C_5H_6O_2$: f50
$C_5H_6O_3$: g15, h156
$C_5H_6O_4$: c284, m253
$C_5H_6O_4S_3$: b156
C_5H_6S: m441, m442
C_5H_7BN: b244
$C_5H_7BrO_3$: e91
$C_5H_7ClO_2$: c205, d581
$C_5H_7ClO_3$: m189, m190, m195
C_5H_7N: m417, p51, p52
C_5H_7NO: e31, f51
$C_5H_7NO_2$: c324, e115
$C_5H_7N_3$: a224, d58
$C_5H_7N_3O$: a188
C_5H_8: c401, d424, m157, m178, p15, p16, p17, p18, p58
$C_5H_8Br_2O_2$: e122
$C_5H_8N_2$: d626, d684, e191, p283
$C_5H_8N_2O_2$: d622
$C_5H_8N_4O_{12}$: p22
C_5H_8O: c399, c410, d364, e6, m179
$C_5H_8O_2$: a74, c334, d532, e60, g16, i95, m65, m168, m169, m170, m200, m225, m300, p33, p34, p207, v2, v3, v10, v14
$C_5H_8O_3$: e237, h121, m123, o63
$C_5H_8O_4$: d547, g14, m278
C_5H_9Br: b313, b365
$C_5H_9BrO_2$: b364, e93, e94, m155
C_5H_9Cl: c93
C_5H_9ClO: c206, d681, m186, p45, t75, t351
C_5H_9ClOS: c238
$C_5H_9ClO_2$: b538, c237, e110, e111, i68, i107, m193
C_5H_9N: d683, m185, p35
C_5H_9NO: b565, b566, c400, d531, e53, e234, m419, m461
$C_5H_9NO_2$: d523, f39, m130, p187
$C_5H_9NO_4$: g12
C_5H_{10}: c396, m165a, m166, m167, p48, p49, p50
$C_5H_{10}Br_2$: d117, d118
$C_5H_{10}ClNO$: d348
$C_5H_{10}Cl_2$: d209
$C_5H_{10}Cl_2$: d251
$C_5H_{10}I_2$: d453
$C_5H_{10}NO_3P$: d293a
$C_5H_{10}N_2$: d548
$C_5H_{10}N_2O$: d627
$C_5H_{10}N_2O_3$: g13
$C_5H_{10}N_2O_4S_2$: c412
$C_5H_{10}O$: a85, c398, d653, d677, e252, m165, m171, m172, m173, m180, m181, m429, p28, p42, p43, t83
$C_5H_{10}OS$: m439
$C_5H_{10}O_2$: b557, c398, d521, d679, e252, h147, h164, i69, i99, m86, m182, m183, m184, m237, m290, m353, p38, p222, t71, t349
$C_5H_{10}O_2S$: e197, e222, m316, m431
$C_5H_{10}O_3$: d349, d520, e194, m75, m282, m307
$C_5H_{10}O_4$: b201, m72
$C_5H_{10}O_5$: a300, r9, x8
$C_5H_{11}Br$: b362, b363, b387, b388
$C_5H_{11}BrO$: b322
$C_5H_{11}BrO_2$: b320
$C_5H_{11}Br_2O$: b148
$C_5H_{11}Br_2O_2$: b150
$C_5H_{11}Cl$: c109, c150, c169a, c170, c204a
$C_5H_{11}ClO$: c110
$C_5H_{11}Cl_2N$: b164
$C_5H_{11}I$: i47

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

C_6H_6IN: i22
$C_6H_6NO_6$: n20
$C_6H_6N_2O$: e49, p259, p260, p264
$C_6H_6N_2O_2$: n23, n24, n25
$C_6H_6N_2O_3$: a238, a239, a240, m94
$C_6H_6N_4O_4$: d721, n53
C_6H_6O: p65
C_6H_6OS: a57, m443
$C_6H_6O_2$: a44, c21, d428, d429, d430, h86, m258, r2
$C_6H_6O_2S$: b21, t152
$C_6H_6O_3$: b34, m259a, t317, t318
$C_6H_6O_3S$: b23
$C_6H_6O_4$: d529
$C_6H_6O_6$: p206
C_6H_6S: t156
$C_6H_7AsO_3$: b12
$C_6H_7BO_2$: b13
$C_6H_7ClN_2$: c216, c217
C_6H_7N: a293, a294, m409, m410, m411
C_6H_7NO: a252, a253, a254, h155, m113, p273, p274
$C_6H_7NO_2$: m414
$C_6H_7NO_2S$: b22
$C_6H_7NO_3S$: a115, a116, a117, s25
C_6H_7NS: a287
$C_6H_7N_3O_2$: n65, n66, n67
$C_6H_7O_2P$: p138
$C_6H_7O_3P$: p139
$C_6H_8AsNO_3$: a113
$C_6H_8Br_2O_2$: d107
$C_6H_8Br_3O$: t205
$C_6H_8ClN_3O_4S_2$: a137
$C_6H_8Cl_2O_2$: m228
$C_6H_8N_2$: a218, a219, a220, a221, a222, a223, d284, m263, p104, p105, p106, p117
$C_6H_8N_2O$: a204, o69
$C_6H_8N_2O_2S$: b26, s24
$C_6H_8N_2O_3$: d561a
C_6H_8O: c371, d609, d620, h38
$C_6H_8O_2$: b451, c360, h40, m223
$C_6H_8O_3$: a36, a311, d599, f47
$C_6H_8O_4$: d598, d608, d629, d630
$C_6H_8O_6$: a302, g11, i61
$C_6H_8O_7$: c289
C_6H_9Br: b312
$C_6H_9BrO_3$: b285
$C_6H_9ClO_3$: e106, e107
$C_6H_9F_3O_2$: b605
C_6H_9NO: o62, v17
C_6H_9NOS: m433
$C_6H_9NO_2$: b540
$C_6H_9NO_3$: m78, n49
$C_6H_9N_3$: a156
$C_6H_9N_3O_2$: a157, c317, h83
C_6H_{10}: c368, d566, h39, h82, m356
$C_6H_{10}Br_2$: d89
$C_6H_{10}N_2$: e211, i114, p181
$C_6H_{10}N_2O_2$: c361
$C_6H_{10}N_2O_4$: d338
$C_6H_{10}N_2O_5$: a14
$C_6H_{10}N_4$: p27
$C_6H_{10}O$: c366, c370, d31, d362, e12, h77, m224, m368, m370, m372
$C_6H_{10}O_2$: a91, c397, d422, e114, e119, e142, e199, h60, h69, h74, h75, m369
$C_6H_{10}O_3$: d501, e58, e143, h126, h177, m402, p214
$C_6H_{10}O_4$: d385, d634, d691, e22, e137, h54, m276, m303
$C_6H_{10}O_4S$: t146
$C_6H_{10}O_4S_2$: d794, e136
$C_6H_{10}O_5$: d386
$C_6H_{10}O_6$: d699, g7
$C_6H_{10}S$: d34
$C_6H_{11}Br$: b311
$C_6H_{11}BrO$: b424
$C_6H_{11}BrO_2$: b279, b347, b529, e85, e86, e89
$C_6H_{11}BrO_4$: d346
$C_6H_{11}Cl$: c91
$C_6H_{11}ClO$: h72
$C_6H_{11}ClO_2$: b535, c82, e98
$C_6H_{11}I$: i28
$C_6H_{11}N$: d30, h61, m361
$C_6H_{11}NO$: c367, e260, f40, m388, o61, t379
$C_6H_{11}NO_2$: e66
C_6H_{12}: c347, d572a, d573, d574, e95a, h73, m222
$C_6H_{12}Br_2$: d94, d106
$C_6H_{12}ClNO$: c133
$C_6H_{12}Cl_2$: d217, d219, d234
$C_6H_{12}Cl_2O$: b166
$C_6H_{12}Cl_2O_2$: b161, d169
$C_6H_{12}Cl_3O_3P$: t437
$C_6H_{12}Cl_3O_4P$: t436
$C_6H_{12}F_3NOSi$: m457
$C_6H_{12}NO_3P$: d294
$C_6H_{12}N_2$: d61, d325, t279
$C_6H_{12}N_2S$: b183, t119
$C_6H_{12}N_2S_4$: t120
$C_6H_{12}N_2Si$: t396
$C_6H_{12}N_2Zn$: d601
$C_6H_{12}N_4$: h49
$C_6H_{12}O$: a96, b609, c365, d572, e11, e98, h51, h70, h71, h76, i78, m367, m430
$C_6H_{12}O_2$: b465, b501, b502, b503, c359, d576, d577, e99, e100, e192, e209, e213, h64, h150, i63, m235, m312, m362, m363, m456, p244, t84
$C_6H_{12}O_3$: d525, e42, e179, e182, i116, p2, p237, t70
$C_6H_{12}O_4$: e149
$C_6H_{12}O_4Si$: d27
$C_6H_{12}O_6$: f41, g1, g8, i19, m11, s6
$C_6H_{12}O_7$: g6
$C_6H_{12}S$: c364
$C_6H_{13}Br$: b346
$C_6H_{13}BrO_2$: b317
$C_6H_{13}Cl$: c149
$C_6H_{13}ClO$: c150
$C_6H_{13}ClO_2$: c96
$C_6H_{13}ClO_3$: c124
$C_6H_{13}I$: i36
$C_6H_{13}N$: c375, e202, h48, m383, m384, m385, m386
$C_6H_{13}NO$: d314, d637, e223, h133, h152
$C_6H_{13}NO_2$: a182, a183, h127, i88, L5, L6, m233
$C_6H_{13}NO_4$: b199
$C_6H_{13}NO_5$: t441
C_6H_{14}: d567, d568, h52, m357, m358
$C_6H_{14}ClN$: d328
$C_6H_{14}Cl_4OSi_2$: b175
$C_6H_{14}NO_2$: b213
$C_6H_{14}N_2$: a214, c354, d43, d44, d671, e245
$C_6H_{14}N_2O$: a172, h129
$C_6H_{14}N_2O_2$: L13
$C_6H_{14}N_4O_2$: a301
$C_6H_{14}O$: b554, d476, d570, d570a, d571, d786, e95, h66, h67, h68, m364, m365, m366
$C_6H_{14}OSi$: a93

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

$C_6H_{14}O_2$: b493, d303, d304, d569, e138, e219, h55, h56, h57, m82, m360, p220
$C_6H_{14}O_2S$: d789
$C_6H_{14}O_3$: b204, b214, d305, d779, e41, e183, h63, h176, t321, t341
$C_6H_{14}O_4$: t280
$C_6H_{14}O_4S$: d788
$C_6H_{14}O_4S_2$: b459
$C_6H_{14}O_6$: d824, m10, s5
$C_6H_{14}O_6S_2$: b210
$C_6H_{14}S$: b557, h62
$C_6H_{14}Si$: a101
$C_6H_{15}Al$: t273
$C_6H_{15}AlI$: d322
$C_6H_{15}AlO$: d321
$C_6H_{15}As$: t276
$C_6H_{15}B$: t277
$C_6H_{15}ClGe$: c260
$C_6H_{15}ClO_3Si$: c240
$C_6H_{15}ClSi$: b551, c261
$C_6H_{15}Ga$: t286
$C_6H_{15}In$: t288
$C_6H_{15}N$: d468, d575, d777, e97, h81, m371, t274
$C_6H_{15}NO$: a184, a211, a212, b513, b553, d327, d364, i98
$C_6H_{15}NO_2$: d306, d540, e125
$C_6H_{15}NO_3$: t266
$C_6H_{15}N_3$: a174
$C_6H_{15}O_3B$: t268
$C_6H_{15}O_3P$: d480, t294
$C_6H_{15}O_3PS$: t298
$C_6H_{15}O_4P$: t292
$C_6H_{15}P$: t293
$C_6H_{15}Sb$: t275
$C_6H_{16}Br_2OSi_2$: b149
$C_6H_{16}Cl_2OSi_2$: b167
$C_6H_{16}N_2$: d367, h53, m359, t108
$C_6H_{16}OSi$: p221
$C_6H_{16}O_2Si$: d301
$C_6H_{16}O_3SSi$: m24
$C_6H_{16}O_3Si$: t269, t342
$C_6H_{16}Si$: t297
$C_6H_{17}NO_3Si$: a274, t344
$C_6H_{17}N_3$: i9
$C_6H_{18}ClN_3Si$: c268a
$C_6H_{18}N_2Si$: b179
$C_6H_{18}N_3OP$: h50
$C_6H_{18}N_4$: t285, t434
$C_6H_{18}OSi_2$: h47
$C_6H_{18}O_3Si_3$: h45
$C_6H_{19}NOSi_2$: b233
$C_6H_{19}NSi_2$: h46

C_7

$C_7H_3BrClF_3$: b297
$C_7H_3BrF_3NO$: b380
$C_7H_3ClF_3NO_2$: c199, c200
$C_7H_3ClN_2O_5$: d714
$C_7H_3Cl_2F_3$: d206, d207
$C_7H_3Cl_2NO$: d259
$C_7H_3Cl_3O$: d208, d209
$C_7H_4BrF_3$: b268, b269
$C_7H_4Br_4O$: t15
C_7H_4ClFO: f14, f15
$C_7H_4ClF_3$: c60, c61, c62
C_7H_4ClN: c54, c55
C_7H_4ClNO: c219, c220
$C_7H_4ClNO_3$: n39, n40
$C_7H_4ClNO_4$: c195, c196, c197
$C_7H_4Cl_2O$: c64, c65, d194, d195
$C_7H_4Cl_2O_2$: d202, d203, d204
$C_7H_4Cl_3F$: t238
$C_7H_4Cl_4$: c58, c59
$C_7H_4F_3NO_2$: n86, n87
$C_7H_4I_2O_3$: h113
$C_7H_4N_2O_2$: n38
$C_7H_4N_2O_6$: d713
$C_7H_4N_2O_7$: d722, h114
$C_7H_4O_3S$: h105
$C_7H_4O_4S$: s27
C_7H_5BrO: b65
$C_7H_5BrO_2$: b266, b265
$C_7H_5BrO_3$: b419
$C_7H_5ClF_3N$: a142, a143
C_7H_5ClO: b66, c43, c44, c45
$C_7H_5ClO_2$: c51, c52, c53, p99
$C_7H_5ClO_3$: c207, c245, c246
$C_7H_5Cl_2F$: c139
$C_7H_5Cl_2NO$: d196, d197
$C_7H_5Cl_3$: t251, t252, t253, t254
C_7H_5FO: b68, f9, f10
$C_7H_5FO_2$: f12, f13
$C_7H_5F_3$: t311
$C_7H_5F_3N_2O_2$: a237
$C_7H_5F_3O$: t304
$C_7H_5F_4N$: a179
$C_7H_5IO_2$: i25
$C_7H_5IO_3$: i51
$C_7H_5I_2NO_2$: a154
C_7H_5N: b51
C_7H_5NO: b62, p124
$C_7H_5NO_3$: n26, n27
$C_7H_5NO_3S$: s1
$C_7H_5NO_4$: n35, n36, n37, p268, p269, p270
$C_7H_5NO_5$: h163
C_7H_5NS: b59, p125
$C_7H_5NS_2$: m17, m19
$C_7H_5N_3O_2$: a234, n34, n55
$C_7H_5N_3O_2S$: a236
$C_7H_5N_3O_6$: t405
C_7H_6BrClO: b300
$C_7H_6BrNO_2$: n44
$C_7H_6BrNO_3$: h156
$C_7H_6Br_2$: b271, d132
$C_7H_6Br_2O$: d111
C_7H_6ClF: c143, c144, f16
C_7H_6ClNO: c46
$C_7H_6ClNO_2$: a138, a139, c202, c203, n45
$C_7H_6Cl_2$: c69, c70, d273, d274, d275, d276
$C_7H_6F_3N$: a126, a127, a128, t310
$C_7H_6FNO_2$: f24
$C_7H_6INO_2$: a199
$C_7H_6N_2$: a121, a122, a123, b39
$C_7H_6N_2O_3$: n28, n29
$C_7H_6N_2O_4$: a233, d723, d724
$C_7H_6N_2O_5$: d715, d716
$C_7H_6N_2S$: a125
$C_7H_6N_4O_2$: t134
C_7H_6O: b3
C_7H_6OS: t139
$C_7H_6O_2$: b44, h94, h95, h96, m251
$C_7H_6O_2S$: m18
$C_7H_6O_3$: d427, f46, h99, h100, h101
$C_7H_6O_4$: d431, d432, d433, d434
$C_7H_6O_5$: t319
$C_7H_6O_6S$: s31
C_7H_7Br: b85, b429, b430, b431
C_7H_7BrO: b259, b260, b270, b357, b358, b359
C_7H_7BrS: b425
C_7H_7Cl: b90, c255, c256, c257
$C_7H_7ClNNaO_2S$: c258
$C_7H_7ClN_4O_2$: c253
C_7H_7ClO: c66, c160, c176, c177
$C_7H_7ClO_2S$: t177
$C_7H_7ClO_3S$: m56

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

C_7H_7ClS: c73
$C_7H_7Cl_3Si$: b128
C_7H_7F: f27, f28, f29
C_7H_7FO: f19, f20
$C_7H_7FO_2S$: t178
C_7H_7I: i53, i54, i55
C_7H_7N: v15, v16
C_7H_7NO: a53, a54, a55, b4, f35
$C_7H_7NO_2$: a118, a119, a120, h97, h98, m412, m413, n83, n84, n85
$C_7H_7NO_3$: a280, a281, m92, m339, m340, n41, n42, n43
$C_7H_7NO_4S$: c17
$C_7H_7N_3$: a197, a198
C_7H_8: b134, c344, t166
C_7H_8BrN: b360
C_7H_8ClN: c37, c67, c68, c163, c164, c165, c166, c167
C_7H_8ClNO: c158, c159
$C_7H_8ClNO_2$: c19
$C_7H_8ClNO_2S$: c248
$C_7H_8Cl_2Si$: d239
$C_7H_8N_2$: h102
$C_7H_8N_2O$: a112, b71, p167
$C_7H_8N_2O_2$: d40, h149, h170, m326, m327, m328, m329, m330, m415
$C_8H_8N_2O_3$: m89, m90, m91
$C_7H_8N_2S$: p158
$C_7H_8N_4O_2$: t133
C_7H_8O: b78, c303, c304, c305, m55
$C_7H_8O_2$: d438, h106, m97, m98, m99, m280
$C_7H_8O_2S$: t172
$C_7H_8O_3$: e155, f49, m314
$C_7H_8O_3S$: m139, t176
C_7H_8S: b106, m379, t142
$C_7H_9BrO_2$: e84
C_7H_9N: b79, d685, d686, d687, d688, d689, e256, e257, e258, m134, t180, t181, t182
C_7H_9NO: a213, b101, h132, m48, m49, m50
$C_7H_9NO_2$: d524
$C_7H_9NO_2S$: t173, t174
$C_7H_9NO_3S$: a205, a206, a288
C_7H_9NS: m436
C_7H_{10}: b135
$C_7H_{10}ClN_3O$: g4
$C_7H_{10}N_2$: a177, a178, d59, d60, d287, d551, t167, t168, t169, t170
$C_7H_{10}N_2O$: o66
$C_7H_{10}N_2O_2$: e212, m242
$C_7H_{10}N_2O_2S$: t175
$C_7H_{10}O$: d294, m67, n108, t67
$C_7H_{10}O_2$: a40, c402
$C_7H_{10}O_3$: e17, e144, m354, t367
$C_7H_{10}O_4$: d29, d596, p208
$C_7H_{10}O_5$: d528
$C_7H_{11}Br$: b383
$C_7H_{11}BrO_4$: d346
$C_7H_{11}ClO$: c351
$C_7H_{11}N$: c350
$C_7H_{11}NO$: c381, h112
$C_7H_{11}NO_2$: a52, b539
$C_7H_{11}NO_3$: m83
$C_7H_{11}NO_5$: a45
$C_7H_{11}NS$: c382
C_7H_{12}: c345, h20, m215, m216, n107
$C_7H_{12}N_2O$: m464
$C_7H_{12}O$: b506, c348, c352, c369, m212, m213, m214
$C_7H_{12}O_2$: a80, b507a, b508, c353, d420, e126, i65
$C_7H_{12}O_3$: e43, e201, e226, h178, t73
$C_7H_{12}O_4$: d378, d379, d636, d656, h7, m76, m277, t125
$C_7H_{12}O_6Si$: m448
$C_7H_{13}Br$: b310, b367
$C_7H_{13}BrO_2$: b390, e92
$C_7H_{13}ClO$: h17
$C_7H_{13}N$: a245
$C_7H_{13}NO$: a307, b507, c380
$C_7H_{13}NO_2$: d541
$C_7H_{13}NO_3$: d418
C_7H_{14}: c341, e118a, h18, h18a, h18b, m202
$C_7H_{14}ClN$: c134
$C_7H_{14}N_2$: d475
$C_7H_{14}N_2O$: a272
$C_7H_{14}N_2O_2$: e246
$C_7H_{14}O$: c342, c384, d655, d658, h3, h14, h15, h16, m205, m206, m207, m208, m209, m210, m211, m271
$C_7H_{14}O_2$: b559, b593, b594, d312, e128, e207, e208, e239, h9, i74, i91, i106, m270, p53, p228
$C_7H_{14}O_2S$: b569
$C_7H_{14}O_3$: b567, e130, e151
$C_7H_{14}O_6$: m262
$C_7H_{15}Br$: b343, b344
$C_7H_{15}Cl$: c147
$C_7H_{15}ClO_2$: c97
$C_7H_{15}I$: i34
$C_7H_{15}N$: c362, d672, e247, e248, m218, m219, m220
$C_7H_{15}NO$: e186, h131, h134, m387, p182, p183
$C_7H_{15}NO_2$: p286
$C_7H_{15}NO_3$: m467
$C_7H_{15}O_5P$: t296
C_7H_{16}: d654, e238, h6, t361
$C_7H_{16}BrNO_2$: a38
$C_7H_{16}ClNO_2$: a39
$C_7H_{16}N_2$: a210, a271, m308, t392
$C_7H_{16}N_2S$: d482
$C_7H_{16}O$: d657, h10, h11, h12, t362
$C_7H_{16}O_2$: b498, b499, d311, d393, m405
$C_7H_{16}O_2Si$: d310
$C_7H_{16}O_3$: d784, t290
$C_7H_{16}O_4$: t92, t284
$C_7H_{16}S$: h8
$C_7H_{17}N$: h19, m272
$C_7H_{17}NO$: b500, d332, d333
$C_7H_{17}NO_2$: b515, d331
$C_7H_{17}NO_5$: m261
$C_7H_{18}N_2$: d334, d392, t116
$C_7H_{18}N_2O$: b180
$C_7H_{18}N_2O_2$: a270
$C_7H_{18}N_2O_4Si$: t348
$C_7H_{18}O_2Si$: b607
$C_7H_{18}O_3Si$: b606, i77, m451
$C_7H_{19}NOSi_2$: b232
$C_7H_{19}NSi$: d404
$C_7H_{19}N_3$: d52
$C_7H_{20}N_2OSi_2$: b236
$C_7H_{22}O_4Si_3$: h5

C_8

$C_8Br_4O_3$: t17
$C_8Cl_4O_3$: t40
C_8D_{10}: e73
$C_8F_{18}O_2S$: p59
$C_8HCl_4NO_2$: t39
$C_8H_3NO_5$: n72
$C_8H_4BrNO_2$: b348
$C_8H_4Cl_2O_2$: b15, b16, p172
$C_8H_4Cl_2O_4$: d261
$C_8H_4Cl_6$: b225
$C_8H_4F_6$: b229
$C_8H_4N_2$: d282, d283

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

$C_8H_{16}O$: c378, c391, d500, d590, d591, e118, e158, m268, o36, o37, o38, o43
$C_8H_{16}O_2$: b531, c357, c390, e160, e161, h79, i70, m266, o30, p239
$C_8H_{16}O_3$: b497, e181
$C_8H_{16}O_4$: c313, e37, t124
$C_8H_{17}Br$: b385
$C_8H_{17}Cl$: c204
$C_8H_{17}Cl_3Si$: o48
$C_8H_{17}I$: i44
$C_8H_{17}N$: b597, c394, d593, d594
$C_8H_{17}NO_3$: e173
$C_8H_{17}O_5P$: t295
C_8H_{18}: d616a, e158a e214, e215, o23, t100, t380, t381, t382
$C_8H_{18}AlCl$: d455
$C_8H_{18}ClNO_2$: a49
$C_8H_{18}Cl_2Sn$: d177
$C_8H_{18}F_3NOSi_2$: b235
$C_8H_{18}N_2$: c349
$C_8H_{18}N_2O_4S$: h130
$C_8H_{18}N_2O_6S_2$: p179
$C_8H_{18}O$: d148, d458, e162, m267, o32, o33, o34, o35, o66a
$C_8H_{18}OSi_2$: d799
$C_8H_{18}OSn$: d180
$C_8H_{18}O_2$: b494, d159, d618, e159, o26, o27, t383
$C_8H_{18}O_2S$: d173
$C_8H_{18}O_3$: b186, b495, t289
$C_8H_{18}O_3S$: d172
$C_8H_{18}O_3Si$: t272
$C_8H_{18}O_4$: b211, t282
$C_8H_{18}O_4S$: d169
$C_8H_{18}O_5$: t51
$C_8H_{18}S$: d170, d171, o29
$C_8H_{18}S_2$: b154, b155, d146, d147
$C_8H_{18}Si_2$: b231
$C_8H_{19}Al$: d456
$C_8H_{19}N$: d139, d140, d457, d477, d619, e166, o44, t103
$C_8H_{19}NO$: d413
$C_8H_{19}NO_2$: b549, d299, d300
$C_8H_{19}O_3P$: d164
$C_8H_{20}BrN$: t49
$C_8H_{20}ClN$: t50
$C_8H_{20}Ge$: t58
$C_8H_{20}N_2$: o24, t101, t102
$C_8H_{20}N_2O_2S$: t61
$C_8H_{20}O_3Si$: e270
$C_8H_{20}O_4Si$: t48
$C_8H_{20}O_4Ti$: t163
$C_8H_{20}Pb$: t59
$C_8H_{20}Si$: t60
$C_8H_{20}Sn$: t63
$C_8H_{21}NOSi_2$: b230
$C_8H_{21}NO_2Si$: a269, d308
$C_8H_{22}B$: b241
$C_8H_{22}N_2O_3Si$: a166, t346
$C_8H_{22}N_4$: b145
$C_8H_{22}O_2Si_2$: b234
$C_8H_{23}N_5$: t56
$C_8H_{24}Cl_2O_3Si_4$: d250
$C_8H_{24}O_2Si_3$: o22
$C_8H_{24}O_4Si_4$: o21
$C_8H_{35}N$: d728

C_9

$C_9H_2Cl_6O_3$: h28
$C_9H_3Cl_3O_3$: b33
$C_9H_4O_5$: b32
$C_9H_5BrClNO$: b304
$C_9H_5Br_2NO$: d108
C_9H_5ClINO: c152
$C_9H_5Cl_2N$: d270
C_9H_6BrN: b418
C_9H_6ClNO: c153
$C_9H_6INO_4S$: h137
$C_9H_6N_2O_2$: t171
$C_9H_6O_2$: b55, c292
$C_9H_6O_3$: h111
$C_9H_6O_4$: i13
$C_9H_6O_6$: b29, b30, b31
C_9H_7BrO: b309
C_9H_7ClO: c280
$C_9H_7ClO_2$: c90
C_9H_7N: i133, q3
C_9H_7NO: h184
$C_9H_7NO_3$: h151, m289
$C_9H_7NO_4$: n50
$C_9H_7NO_4S$: h185
$C_9H_7N_3O_4S_2$: a242
C_9H_8: i14
$C_9H_8Cl_2O_3$: d258
$C_9H_8N_2$: m423, p120
$C_9H_8N_2O_6$: e129
C_9H_8O: c278, i12
$C_9H_8O_2$: c279, d417, v6
$C_9H_8O_3$: h109
$C_9H_8O_3S$: p247
$C_9H_8O_4$: p127
C_9H_9BrO: b412
$C_9H_9BrO_2$: b86
C_9H_9Cl: v7
C_9H_9ClO: c234
$C_9H_9ClO_3$: c213, d498
C_9H_9N: d564, m287
C_9H_9NO: m103, m104, p134
$C_9H_9NO_2$: a9
$C_9H_9NO_3$: a11, a12, b70
$C_9H_9NO_4$: e227
$C_9H_9N_3O$: a260
$C_9H_9N_3O_2S_2$: t137
$C_9H_9N_5$: d53
C_9H_{10}: a78, i10, m425, m426
$C_9H_{10}Br_2$: d109
$C_9H_{10}F_3NO_2$: m135
$C_9H_{10}N$: a196, a197
$C_9H_{10}N_2$: a296, p121
$C_9H_{10}N_2O$: p151
$C_9H_{10}N_2O_2$: p85
$C_9H_{10}N_2O_3$: a129
$C_9H_{10}O$: a94, a95, c282, e14, e72, i11, m124, p147, p148, p149, p209, p217
$C_9H_{10}O_2$: b63, b76, d563, e33, e34, e76, h174, h175, m44, m45, m46, m309, m310, m311, m375, p103, p150, t190
$C_9H_{10}O_3$: d491, d492, e37, e38, e46, e55, e178, e261, f52, m101, m283, m297, m304, m305, p74
$C_9H_{10}O_4$: d496, d492, h135, m292
$C_9H_{11}Br$: b350, b353, b399, b435, b436
$C_9H_{11}BrO$: b413, p75
$C_9H_{11}Cl$: c222
$C_9H_{11}ClO_3S$: c135
$C_9H_{11}N$: a77, c333, m288, t78, t86
$C_9H_{11}NO$: d536, d562, m121, m374, m445
$C_9H_{11}NO_2$: d537, d538, e35, e64, e65, i126, p86
$C_9H_{11}NO_3$: t455
C_9H_{12}: e190, i103, p225, t357, t358, t359, v13
$C_9H_{12}N_2O_4$: a241
$C_9H_{12}N_2O_6$: u18
$C_9H_{12}N_2S$: b111
$C_9H_{12}O$: b98, d632, d633, i127, i128, i129, m373, p145, p146, p240, t385, t386, t387
$C_9H_{12}O_2$: b115, c316, c358, e48, p73, p148, t365, t374

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

$C_9H_{12}O_3$: d499, m204, t332, t333, t334
$C_9H_{12}O_3S$: e263
$C_9H_{12}S$: p144
$C_9H_{13}N$: b595, d565, d706, e80, e203, e264 e265, e266, i101, t355
$C_9H_{13}NO$: b80, m96, n110
$C_9H_{13}NO_2$: a258, b596
$C_9H_{13}N_5$: t191
$C_9H_{14}BrN$: p162
$C_9H_{14}Br_3N$: p165
$C_9H_{14}ClN$: p163
$C_9H_{14}IN$: p164
$C_9H_{14}N_2$: n92, t388
$C_9H_{14}O$: d611, d613, i93, t364
$C_9H_{14}O_2$: m350
$C_9H_{14}O_2Si$: d510
$C_9H_{14}O_3$: b215, t76
$C_9H_{14}O_3Si$: p161
$C_9H_{14}O_5$: d315, d382
$C_9H_{14}O_6$: p200
$C_9H_{14}Si$: p166
$C_9H_{15}N$: t195
$C_9H_{15}NO$: c362
$C_9H_{15}N_3$: t439
C_9H_{16}: m348
$C_9H_{16}N_2$: d62
$C_9H_{16}O$: d612, n103
$C_9H_{16}O_2$: b571, c363, h80, n97
$C_9H_{16}O_3$: b568, b582
$C_9H_{16}O_4$: d368, d371, d478, d614, n93
$C_9H_{16}O_6$: d345
$C_9H_{17}BrO_2$: e87
$C_9H_{17}Cl$: c92
$C_9H_{17}ClO$: n102, t372
$C_9H_{17}ClO_2$: e167
$C_9H_{17}N$: a83, n95
$C_9H_{17}NO_2$: e216, e217
C_9H_{18}: i108, p229, t363
$C_9H_{18}NO$: t115
$C_9H_{18}N_2O$: d550
$C_9H_{18}O$: c385, d616, n99, n100, n101, n104, t370
$C_9H_{18}O_2$: e156, m349, n96
$C_9H_{18}O_3$: d144
$C_9H_{18}O_4$: d785
$C_9H_{19}Br$: b382
$C_9H_{19}BrO_2$: e90
$C_9H_{19}I$: i42
$C_9H_{19}NO$: d151
$C_9H_{19}NO_3Si$: t270
$C_9H_{19}N_2S$: d175
C_9H_{20}: d386a, d613a, e210a, n90, t370a
$C_9H_{20}Cl_2Si$: d238
$C_9H_{20}N_2$: a136, a290
$C_9H_{20}N_2S$: d136
$C_9H_{20}O$: d615, n98, t371
$C_9H_{20}O_2$: b556, n94
$C_9H_{20}O_2Si$: c377
$C_9H_{20}O_3$: d783, t291
$C_9H_{20}O_3Si$: a99
$C_9H_{20}O_4$: t430
$C_9H_{21}Al$: t428
$C_9H_{21}BO_3$: t427, t326
$C_9H_{21}BO_6$: t445
$C_9H_{21}ClO_3Si$: c239
$C_9H_{21}N$: n105, t429
$C_9H_{21}NO_2$: d470, d778
$C_9H_{21}NO_3$: t325
$C_9H_{21}N_3$: t287
$C_9H_{21}O_3P$: t329
$C_9H_{22}N_2$: d387, n91
$C_9H_{22}O_3$: d780, d781
$C_9H_{22}Si$: t330
$C_9H_{23}N_3$: p26
$C_9H_{24}N_4$: b147
$C_9H_{24}O_2Si_3$: m153
$C_9H_{27}BO_3Si_3$: t449
$C_9H_{31}ClO_3Ti$: c254

C_{10}

$C_{10}H_2O_6$: b28
$C_{10}H_4Cl_2O_2$: d243
$C_{10}H_6Br_2O$: d113
$C_{10}H_6Cl_2O$: d242
$C_{10}H_6N_2$: b103
$C_{10}H_6N_2O_4$: d719
$C_{10}H_6N_2O_4S$: d64
$C_{10}H_6O_2$: n11
$C_{10}H_6O_3$: h161
$C_{10}H_6O_8$: b27
$C_{10}H_7Br$: b376
$C_{10}H_7BrO$: b377, b378
$C_{10}H_7Br_2NO$: d112
$C_{10}H_7Cl$: c185, c186
$C_{10}H_7NO_2$: n57, n80, p126
$C_{10}H_7NO_8S_2$: n81
$C_{10}H_8$: a316, d1, n2
$C_{10}H_8BrNO_2$: b339
$C_{10}H_8N_2$: d790
$C_{10}H_8N_2O_4$: b205, f53
$C_{10}H_8O$: n9, n10
$C_{10}H_8O_2$: d439, d440, d441, d442, m199
$C_{10}H_8O_3$: h148
$C_{10}H_8O_3S$: n6, n7
$C_{10}H_8O_4$: d443, d444
$C_{10}H_9N$: a228, a229, m420, m421, m422, n17
$C_{10}H_9NO$: a51, a232
$C_{10}H_9NO_2$: i16
$C_{10}H_9NO_3$: h128
$C_{10}H_9NO_3S$: a230
$C_{10}H_9NO_4S$: a189, a190, a191, a192
$C_{10}H_9NO_6$: d643
$C_{10}H_{10}$: d423
$C_{10}H_{10}BrClO$: b299
$C_{10}H_{10}ClFO$: c121
$C_{10}H_{10}ClNO_2$: c29
$C_{10}H_{10}Cl_2O_3$: d257
$C_{10}H_{10}N_2$: a279, n4, n5
$C_{10}H_{10}N_2O$: m378
$C_{10}H_{10}N_4O_2S$: s21
$C_{10}H_{10}O$: d363, m197, p94, p95
$C_{10}H_{10}O_2$: b63, m66, m198, s2
$C_{10}H_{10}O_3$: b72, m345
$C_{10}H_{10}O_4$: d590, d591, d592, m125, p155, r3
$C_{10}H_{11}BrO$: b375
$C_{10}H_{11}ClO_3$: c212
$C_{10}H_{11}ClO_4$: t336
$C_{10}H_{11}IO_4$: i24
$C_{10}H_{11}N$: p98
$C_{10}H_{11}NO_2$: a24, d514
$C_{10}H_{11}NO_4$: c8, d552a
$C_{10}H_{11}O_2S$: b94
$C_{10}H_{12}$: d292, t80
$C_{10}H_{12}N_2$: a170, b81
$C_{10}H_{12}O$: a89, b77a, b619, e59, e279, i84, i102, m107, m403, p96
$C_{10}H_{12}O_2$: d419, e204, e205, e206, e243, h154, h166, m79, m102, m108, m109, m111, m148, p79, p97, p111, p226
$C_{10}H_{12}O_3$: d487, e47, e195, m306, p71, p102, p235
$C_{10}H_{12}O_4$: d26a, d513, m231, m232, t331
$C_{10}H_{12}O_5$: p245, t335
$C_{10}H_{13}Br$: b280, b351
$C_{10}H_{13}BrO$: b281
$C_{10}H_{13}BrO_2$: b395
$C_{10}H_{13}Cl$: b536, c178
$C_{10}H_{13}NO$: d527, p131
$C_{10}H_{13}NO_2$: m380
$C_{10}H_{13}NS_2$: b95

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

C_{11}

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

$C_{11}H_{24}O$: u7, u8
$C_{11}H_{24}O_6Si$: t444
$C_{11}H_{25}NO_2$: a292
$C_{11}H_{26}N_2$: b555, d166
$C_{11}H_{26}N_2O_6$: b237

C_{12}

$C_{12}H_4Cl_6S_2$: b226
$C_{12}H_6Br_4O_4S$: s28
$C_{12}H_6O_3$: n8
$C_{12}H_6O_{12}$: b20
$C_{12}H_7Cl_6O$: d296
$C_{12}H_8$: a3
$C_{12}H_8Br_2$: d80
$C_{12}H_8Cl_2OS$: b172
$C_{12}H_8Cl_2O_2S$: b171, c223
$C_{12}H_8N_2$: p63
$C_{12}H_8N_2O_4S$: b216
$C_{12}H_8O$: d66
$C_{12}H_8S$: d67
$C_{12}H_9Br$: b273
$C_{12}H_9BrO$: b325, b398
$C_{12}H_9ClO_2S$: c221
$C_{12}H_9N$: c6, d751, n16
$C_{12}H_9NO$: b73, b74, b75
$C_{12}H_9NO_2$: n46, n47
$C_{12}H_9NO_3$: n68, n69
$C_{12}H_9NS$: p67
$C_{12}H_9N_3O_4$: d717
$C_{12}H_{10}$: a2, b138
$C_{12}H_{10}ClN$: a145
$C_{12}H_{10}ClO_3P$: c748
$C_{12}H_{10}ClP$: c118
$C_{12}H_{10}Cl_2Si$: d223
$C_{12}H_{10}Hg$: d758
$C_{12}H_{10}N_2$: a312
$C_{12}H_{10}N_2O$: n79, p90
$C_{12}H_{10}N_2O_2$: n51
$C_{12}H_{10}N_3O_3P$: d764
$C_{12}H_{10}O$: d753, m322, m323, p135, p136
$C_{12}H_{10}OS$: d772
$C_{12}H_{10}O_2$: d436, h89, n14, n15
$C_{12}H_{10}O_2S$: d771, t145
$C_{12}H_{10}O_3$: n12
$C_{12}H_{10}O_3S$: b142
$C_{12}H_{10}O_4$: q1
$C_{12}H_{10}O_4S$: s30
$C_{12}H_{10}S$: d770
$C_{12}H_{10}S_2$: d750
$C_{12}H_{10}Se_2$: d749
$C_{12}H_{11}N$: a130, a131, b122, b123, d743
$C_{12}H_{11}NO$: h115, n13, p70
$C_{12}H_{11}N_3$: p88
$C_{12}H_{11}O_3P$: d763
$C_{12}H_{12}N_2$: b140, d757, p137
$C_{12}H_{12}N_2O$: o68
$C_{12}H_{12}N_2O_2$: b40
$C_{12}H_{12}N_2O_2S$: d47, d48
$C_{12}H_{12}O$: e50
$C_{12}H_{12}O_2Si$: d769
$C_{12}H_{12}O_3$: e78
$C_{12}H_{12}O_6$: t193, t360
$C_{12}H_{13}N$: t68
$C_{12}H_{13}N_3$: d34
$C_{12}H_{13}NO_3S$: p272
$C_{12}H_{14}$: d467
$C_{12}H_{14}N_2$: d46
$C_{12}H_{14}N_4O_2S$: s22
$C_{12}H_{14}O$: b525
$C_{12}H_{14}O_3$: e179
$C_{12}H_{14}O_4$: d391
$C_{12}H_{15}NO$: b121
$C_{12}H_{15}N_3O_3$: t196
$C_{12}H_{15}N_3O_4S$: d42
$C_{12}H_{16}$: b598, c376, m221
$C_{12}H_{16}O_2$: p64
$C_{12}H_{16}O_3$: d298
$C_{12}H_{17}N$: b120
$C_{12}H_{17}NO$: d402
$C_{12}H_{18}$: c338, d473, d474, p116, t453
$C_{12}H_{18}Cl_2N_4OS$: t135
$C_{12}H_{18}N_2$: p186
$C_{12}H_{18}N_2O_2$: i94
$C_{12}H_{18}O$: b552, d479, e4
$C_{12}H_{18}O_2$: b550
$C_{12}H_{18}O_3$: o41
$C_{12}H_{18}O_4$: b463, h58
$C_{12}H_{19}N$: d471
$C_{12}H_{20}O_2$: b202, b296, e112, g3, L12
$C_{12}H_{20}O_3Si$: p160
$C_{12}H_{20}O_4$: d154
$C_{12}H_{20}O_4Sn$: d179
$C_{12}H_{20}O_7$: t278
$C_{12}H_{21}N$: t446
$C_{12}H_{21}NO_3Si$: t345
$C_{12}H_{21}N_3$: t429
$C_{12}H_{22}$: c339, d288
$C_{12}H_{22}BCl$: c95
$C_{12}H_{22}N_2O_8$: d45
$C_{12}H_{22}O$: c337, e5
$C_{12}H_{22}O_2$: d811, e172, m14
$C_{12}H_{22}O_3$: h65
$C_{12}H_{22}O_4$: d168, d384, d597, d787, d805
$C_{12}H_{22}O_6$: d174
$C_{12}H_{22}O_{11}$: L3, L4, m7, s20
$C_{12}H_{23}N$: d289
$C_{12}H_{23}NO$: a308, o47
$C_{12}H_{24}$: d813
$C_{12}H_{24}Cl_2$: d224
$C_{12}H_{24}O$: c326, d817, e8, m459
$C_{12}H_{24}O_2$: d809, e120
$C_{12}H_{24}O_6$: c314
$C_{12}H_{25}Br$: b327
$C_{12}H_{25}Cl$: e119
$C_{12}H_{25}Cl_3Si$: d821
$C_{12}H_{25}I$: i30
$C_{12}H_{25}N$: c340
$C_{12}H_{25}N_3$: i6
$C_{12}H_{26}$: d803
$C_{12}H_{26}O$: d414, d810
$C_{12}H_{26}O_2$: d806, d807
$C_{12}H_{26}O_3$: b151
$C_{12}H_{26}O_4$: d460, t91
$C_{12}H_{26}O_3S$: d820
$C_{12}H_{26}O_5$: t53
$C_{12}H_{26}S$: d808
$C_{12}H_{27}Al$: t322
$C_{12}H_{27}B$: t209
$C_{12}H_{27}BO_3$: t207
$C_{12}H_{27}ClSn$: t213
$C_{12}H_{27}N$: d413, d818, t208
$C_{12}H_{27}O_3P$: t212
$C_{12}H_{27}O_4P$: t211
$C_{12}H_{28}BrN$: t130
$C_{12}H_{28}N_2$: d804
$C_{12}H_{28}O_4Si$: t129
$C_{12}H_{28}O_4Ti$: t164, t165
$C_{12}H_{28}Sn$: t215
$C_{12}H_{29}N$: t323
$C_{12}H_{29}N_3$: b196

C_{13}

$C_{13}H_6Cl_2O_2$: h29
$C_{13}H_8ClNO_3$: c198
$C_{13}H_8Cl_2O$: d205
$C_{13}H_8O$: f3
$C_{13}H_8OS$: t162
$C_{13}H_8O_2$: x3
$C_{13}H_9BrO$: b267
$C_{13}H_9ClO$: c56, c57
$C_{13}H_9ClO_2$: c151
C_3H_9N: a60
$C_{13}H_{10}$: f2
$C_{13}H_{10}ClNO$: a140, a141, d745
$C_{13}H_{10}Cl_2$: d221
$C_{13}H_{10}Cl_2O_2$: m243
$C_{13}H_{10}F_2$: b195
$C_{13}H_{10}N_2$: p91

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

$C_{13}H_{10}N_2O_3$: a235
$C_{13}H_{10}O$: b53, x1
$C_{13}H_{10}O_2$: b139, h103, m68, p92
$C_{13}H_{10}O_3$: d435, d747, p154, r5
$C_{13}H_{10}O_4$: t320
$C_{13}H_{10}O_5$: t88
$C_{13}H_{11}Br$: b326
$C_{13}H_{11}Cl$: c116
$C_{13}H_{11}N$: b102
$C_{13}H_{11}NO$: a124, b5
$C_{13}H_{11}NO_3$: p87
$C_{13}H_{12}$: d759
$C_{13}H_{12}NO_2$: b112
$C_{13}H_{12}N_2$: b54, d754
$C_{13}H_{12}N_2O$: d775
$C_{13}H_{12}N_2S$: d774, t141
$C_{13}H_{12}N_4O$: d746, p89
$C_{13}H_{12}N_4S$: d773
$C_{13}H_{12}O$: d760, h116, h117, m63, p76
$C_{13}H_{12}O_2$: m320
$C_{13}H_{12}O_4$: d32
$C_{13}H_{12}S$: b118
$C_{13}H_{13}ClSi$: c117
$C_{13}H_{13}N$: d761, m238, p93
$C_{13}H_{13}NO_2$: t187
$C_{13}H_{13}N_3$: d755
$C_{13}H_{14}N_2$: d35, m249
$C_{13}H_{14}N_2O_3$: a59
$C_{13}H_{14}N_4O$: d746
$C_{13}H_{15}NO$: i96
$C_{13}H_{16}O_3$: e79
$C_{13}H_{16}O_4$: d389
$C_{13}H_{17}NO_2$: e82
$C_{13}H_{18}O_3$: b117
$C_{13}H_{18}O_5$: t267
$C_{13}H_{20}$: p115
$C_{13}H_{20}O$: i58, i59
$C_{13}H_{22}ClN$: b130
$C_{13}H_{22}N_2$: d290
$C_{13}H_{22}O_3Si$: b129
$C_{13}H_{24}O_2$: e273, i86
$C_{13}H_{24}O_4$: d337
$C_{13}H_{26}$: t265
$C_{13}H_{26}N_2$: m246, t369
$C_{13}H_{26}O$: t263, t264
$C_{13}H_{26}O_2$: e232, t262
$C_{13}H_{27}Br$: b433
$C_{13}H_{28}$: t261
$C_{13}H_{28}O_4$: t431
$C_{13}H_{29}Cl$: c250
$C_{13}H_{29}NO_4$: b176
$C_{13}H_{30}OSn$: t216

C_{14}

$C_{14}H_6Cl_2O_2$: d193
$C_{14}H_7ClO_2$: c41, c42
$C_{14}H_8O_2$: a298
$C_{14}H_8O_4$: d426
$C_{14}H_9Br$: b391
$C_{14}H_9ClO_3$: c63
$C_{14}H_9Cl_5$: b173
$C_{14}H_9NO_2$: a108, a109
$C_{14}H_{10}$: a297, d742, p62
$C_{14}H_{10}ClNO_3$: a144
$C_{14}H_{10}Cl_2O_4$: b168
$C_{14}H_{10}Cl_4$: b169
$C_{14}H_{10}N_2O_2$: d36, d37, d38, d39
$C_{14}H_{10}O_2$: b35
$C_{14}H_{10}O_3$: b45, b64, x2
$C_{14}H_{10}O_4$: b141, d69, b71a
$C_{14}H_{10}O_4S_2$: d796
$C_{14}H_{11}N$: d741, p123
$C_{14}H_{11}NOS$: a50
$C_{14}H_{12}$: d415, s9
$C_{14}H_{12}Cl_2O$: b170
$C_{14}H_{12}N_2O$: b38
$C_{14}H_{12}N_2O_2$: b36
$C_{14}H_{12}O$: a34, d26, m145
$C_{14}H_{12}O_2$: b46, b83, b84, b113, d740
$C_{14}H_{12}O_3$: b37, b100, b125, h144
$C_{14}H_{13}ClO$: c169
$C_{14}H_{13}N$: e104, i9
$C_{14}H_{13}NO$: b82, d739
$C_{14}H_{13}NO_2$: b50
$C_{14}H_{14}$: d752
$C_{14}H_{14}N_2$: a168
$C_{14}H_{14}N_2O$: m240
$C_{14}H_{14}N_2O_3$: a315
$C_{14}H_{14}O$: d73
$C_{14}H_{14}OS$: b223
$C_{14}H_{14}O_2$: b114
$C_{14}H_{14}O_4$: d33
$C_{14}H_{14}S_2$: b222, d72
$C_{14}H_{15}N$: d71
$C_{14}H_{16}N_2O_4$: b207
$C_{14}H_{16}O_2Si$: d503
$C_{14}H_{16}O_4$: d340
$C_{14}H_{18}N_2O_2$: m132
$C_{14}H_{18}O$: p56
$C_{14}H_{18}O_4$: d343
$C_{14}H_{18}O_7$: p21
$C_{14}H_{19}O_3$: d293
$C_{14}H_{22}O$: d160, d161, d162, d163
$C_{14}H_{22}O_2$: d145
$C_{14}H_{22}O_3$: d153
$C_{14}H_{22}O_4$: h59
$C_{14}H_{22}O_6$: t281
$C_{14}H_{22}O_7$: t52
$C_{14}H_{23}N$: d142
$C_{14}H_{23}N_3O_{10}$: d299
$C_{14}H_{26}O_2$: i87
$C_{14}H_{26}O_3$: h10
$C_{14}H_{26}O_4$: d152, d395, d459
$C_{14}H_{27}ClO$: t46
$C_{14}H_{28}$: t47
$C_{14}H_{28}O$: d822
$C_{14}H_{28}O_2$: d815, e272, t44
$C_{14}H_{29}Br$: b423
$C_{14}H_{29}O_4$: b156
$C_{14}H_{30}$: t43
$C_{14}H_{30}O$: t45
$C_{14}H_{30}O_2Sn$: d136
$C_{14}H_{31}N$: d602
$C_{14}H_{32}N_2O_4$: t90
$C_{14}H_{32}OSn$: t214

C_{15}

$C_{15}H_{10}N_2O_2$: m247
$C_{15}H_{10}O_2$: b105, m136, p122
$C_{15}H_{11}NO$: d762
$C_{15}H_{11}NO_2$: m128
$C_{15}H_{12}N_2O_2$: d756
$C_{15}H_{12}O$: c23
$C_{15}H_{12}O_2$: d68
$C_{15}H_{13}NO$: a13
$C_{15}H_{14}O$: d767
$C_{15}H_{14}O_2$: b49, d768, h169
$C_{15}H_{14}O_3$: b116, m239
$C_{15}H_{16}O$: c316a
$C_{15}H_{16}O_2$: e189, i113
$C_{15}H_{17}N$: b96a
$C_{15}H_{17}N_3$: d797
$C_{15}H_{20}O_6$: e184
$C_{15}H_{22}O_3$: d117, e174
$C_{15}H_{22}O_5$: o46
$C_{15}H_{23}N$: b583
$C_{15}H_{24}$: t327
$C_{15}H_{24}O$: d156
$C_{15}H_{26}O_6$: g20
$C_{15}H_{28}O_2$: d816, i112
$C_{15}H_{29}N$: p12
$C_{15}H_{30}N_2$: t368
$C_{15}H_{30}O$: p13
$C_{15}H_{30}O_2$: m428
$C_{15}H_{32}$: p11
$C_{15}H_{32}O_{10}$: t409
$C_{15}H_{33}NO_6$: t443

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

C_{16}

$C_{16}H_{10}$: b52, f1, p255
$C_{16}H_{11}NO_2$: p153
$C_{16}H_{12}N_4O_9S_2$: t5
$C_{16}H_{13}N$: p132, p133
$C_{16}H_{14}$: d744, e71
$C_{16}H_{14}O_2$: b93
$C_{16}H_{14}O_6S$: s29
$C_{16}H_{16}O_2$: b47
$C_{16}H_{16}O_3$: d515
$C_{16}H_{18}ClN_3S$: m248
$C_{16}H_{19}ClSi$: b537
$C_{16}H_{20}N_2$: d74
$C_{16}H_{20}N_2O$: b178
$C_{16}H_{20}O_2Si$: d302
$C_{16}H_{22}O_4$: d165, d410
$C_{16}H_{22}O_{11}$: g9
$C_{16}H_{24}N_2$: d150
$C_{16}H_{26}O_3$: d814
$C_{16}H_{26}O_7$: t54
$C_{16}H_{28}O$: c346
$C_{16}H_{30}O_2$: d819
$C_{16}H_{30}O_4$: b158, d157, d167, d360
$C_{16}H_{32}$: h37
$C_{16}H_{32}O$: e10
$C_{16}H_{32}O_2$: h34
$C_{16}H_{33}Br$: b345
$C_{16}H_{33}Cl$: c148
$C_{16}H_{33}I$: i35
$C_{16}H_{33}NO$: d359
$C_{16}H_{34}$: h4, h31, h36
$C_{16}H_{34}O$: d729, h35
$C_{16}H_{34}O_2$: h32
$C_{16}H_{34}O_4$: b157
$C_{16}H_{34}S$: d720, h33
$C_{16}H_{35}N$: d728, h37
$C_{16}H_{35}O_3P$: b192
$C_{16}H_{36}BF_4N$: t25
$C_{16}H_{36}BrN$: t21
$C_{16}H_{36}BrP$: t29
$C_{16}H_{36}Br_3N$: t26
$C_{16}H_{36}ClN$: t22
$C_{16}H_{36}IN$: t24
$C_{16}H_{36}O_4Si$: t28
$C_{16}H_{36}Sn$: t30
$C_{16}H_{37}NO_4S$: t23

C_{17}

$C_{17}H_{12}O_3$: p118, p119
$C_{17}H_{13}N_3O_5S_2$: p173
$C_{17}H_{15}N_2O$: d355
$C_{17}H_{16}O_4$: d75, p194
$C_{17}H_{18}N_2O_4$: p193
$C_{17}H_{18}O_2$: b589
$C_{17}H_{18}O_3$: b592
$C_{17}H_{18}O_4$: b203
$C_{17}H_{20}N_2O$: b178
$C_{17}H_{20}N_4O_6$: r8
$C_{17}H_{21}NO_4$: b291
$C_{17}H_{22}N_2$: m245
$C_{17}H_{23}NO_3$: a305
$C_{17}H_{24}O_6$: b492
$C_{17}H_{25}NO_2$: m15
$C_{17}H_{27}NO_2$: e170
$C_{17}H_{28}NO$: d149
$C_{17}H_{28}O_7$: d181
$C_{17}H_{34}O_2$: m269a, i131
$C_{17}H_{34}O_4$: b160
$C_{17}H_{36}$: h1
$C_{17}H_{36}O$: h1a
$C_{17}H_{37}N$: m236

C_{18}

$C_{18}H_{12}$: b6, b7
$C_{18}H_{12}N_5O_6$: d766
$C_{18}H_{14}$: t7, t8, t9
$C_{18}H_{14}O_8$: d70
$C_{18}H_{15}As$: t412
$C_{18}H_{15}B$: t414
$C_{18}H_{15}ClSn$: c268, t425
$C_{18}H_{15}N$: t410
$C_{18}H_{15}NO_2$: e116
$C_{18}H_{15}N_3Si$: a310
$C_{18}H_{15}OP$: t421
$C_{18}H_{15}O_3P$: t422
$C_{18}H_{15}O_4P$: t419
$C_{18}H_{15}P$: t420
$C_{18}H_{15}Sb$: t411
$C_{18}H_{16}OSn$: t426
$C_{18}H_{16}O_2$: b520, d280
$C_{18}H_{16}Si$: t423
$C_{18}H_{18}O_3$: e81
$C_{18}H_{20}N_2O_2$: e152
$C_{18}H_{20}O$: b548
$C_{18}H_{20}O_2$: b48
$C_{18}H_{22}$: b182
$C_{18}H_{26}O_6$: e185
$C_{18}H_{30}O$: t210
$C_{18}H_{30}O_2$: o7
$C_{18}H_{32}N_4O_{14}$: d364
$C_{18}H_{32}O_2$: o1
$C_{18}H_{32}O_{16}$: r1
$C_{18}H_{33}ClO$: o13
$C_{18}H_{34}O_2$: o10, o11
$C_{18}H_{34}O_4$: d143
$C_{18}H_{36}$: o8
$C_{18}H_{36}O$: e13, o12
$C_{18}H_{36}O_2$: e157, o5
$C_{18}H_{37}Br$: b384
$C_{18}H_{37}Cl$: c203a
$C_{18}H_{37}Cl_3Si$: o17
$C_{18}H_{37}I$: i43
$C_{18}H_{37}N$: o9
$C_{18}H_{37}NO$: o2
$C_{18}H_{38}$: o3
$C_{18}H_{38}O$: o6
$C_{18}H_{38}S$: o4
$C_{18}H_{39}ClSi$: t315
$C_{18}H_{39}N$: o15, t313
$C_{18}H_{39}O_7P$: t435
$C_{18}H_{40}Si$: t316

C_{19}

$C_{19}H_{15}Br$: b440, t417
$C_{19}H_{15}Cl$: c267, t418
$C_{19}H_{16}$: t415
$C_{19}H_{16}O$: t416
$C_{19}H_{18}BrP$: m458
$C_{19}H_{19}N_7O_6$: f31
$C_{19}H_{20}Br_4O_4$: i110
$C_{19}H_{20}O_4$: b88
$C_{19}H_{22}N_2O$: c276
$C_{19}H_{30}O_5$: m252
$C_{19}H_{31}N$: d24
$C_{19}H_{34}ClN$: b127
$C_{19}H_{36}O_2$: m347
$C_{19}H_{37}NO$: o16
$C_{19}H_{38}O_2$: i109, m346
$C_{19}H_{40}$: n89, t114

C_{20}

$C_{20}H_{10}Br_2O_5$: d105
$C_{20}H_{12}$: b56, b57, d65
$C_{20}H_{12}O_5$: f4
$C_{20}H_{14}O_4$: d765, p66
$C_{20}H_{15}Br$: b439
$C_{20}H_{18}O_2Sn$: t424
$C_{20}H_{19}N_3$: b2
$C_{20}H_{20}BrOP$: h136
$C_{20}H_{32}O_5$: d782
$C_{20}H_{24}N_2O_2$: q2
$C_{20}H_{26}O_4$: d291
$C_{20}H_{27}O_3P$: i90
$C_{20}H_{30}O_2$: a1
$C_{20}H_{30}O_6$: b184
$C_{20}H_{31}N$: d20
$C_{20}H_{34}O_4$: b159
$C_{20}H_{36}O_2$: e229

TABLE 1.14 Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

$C_{20}H_{38}O_2$: e230
$C_{20}H_{38}O_4$: b187
$C_{20}H_{40}$: i2
$C_{20}H_{40}O$: o18
$C_{20}H_{42}$: i1

C_{21} to C_{23}

$C_{21}H_{15}NO$: b143
$C_{21}H_{21}N$: t198
$C_{21}H_{21}O_4P$: t452
$C_{21}H_{22}N_2O_2$: s10
$C_{21}H_{24}O_2$: b144
$C_{21}H_{28}N_2O$: b177
$C_{21}H_{36}O$: p14
$C_{21}H_{40}O_2$: o14
$C_{21}H_{45}N_3O_{12}Si_3$: t448
$C_{22}H_{23}N_3O_9$: a306
$C_{22}H_{26}O$: b181
$C_{22}H_{30}O_2S$: t140
$C_{22}H_{34}O_4$: b547, d463
$C_{22}H_{42}O_8$: b152
$C_{22}H_{44}O_2$: b581, i75
$C_{22}H_{46}$: d801
$C_{22}H_{46}O$: d802
$C_{22}H_{48}N_2$: t27
$C_{23}H_{18}BrO_2P$: c18
$C_{23}H_{26}N_2O_4$: b447
$C_{23}H_{42}O_2$: b581a

C_{24} to C_{29}

$C_{24}H_{16}N_2O_2$: b218
$C_{24}H_{18}$: t413
$C_{24}H_{20}BNa$: t126
$C_{24}H_{20}Sn$: t128
$C_{24}H_{27}NO_2$: e169
$C_{24}H_{38}O_4$: b193, d374, d466, d466a
$C_{24}H_{40}O_5$: c275
$C_{24}H_{46}O_4$: d725, d812
$C_{24}H_{50}$: t41
$C_{24}H_{51}N$: t406
$C_{24}H_{51}O_3P$: t438
$C_{24}H_{54}OSn_2$: b224
$C_{25}H_{30}ClN_3$: c315
$C_{25}H_{34}Cl_6O_4$: b189
$C_{25}H_{48}O_4$: d465
$C_{26}H_{26}N_2O_2S$: b153
$C_{26}H_{42}O_2$: d138
$C_{26}H_{42}O_4$: d464
$C_{26}H_{47}O_3P$: d462
$C_{26}H_{46}O_8$: t312
$C_{26}H_{50}O_4$: b190
$C_{27}H_{42}O$: c274
$C_{27}H_{50}ClN$: b96
$C_{28}H_{31}ClN_2O_3$: r6
$C_{28}H_{32}$: t127
$C_{28}H_{50}O_8$: t314
$C_{28}H_{54}O_6Sn$: b601
$C_{29}H_{44}O_2$: m244
$C_{29}H_{50}O_7$: p20

C_{30} to C_{57}

$C_{30}H_{43}FO_2P$: e188
$C_{30}H_{46}O_2$: e187
$C_{30}H_{50}$: s8
$C_{30}H_{58}O_4S$: d295
$C_{30}H_{62}$: s7
$C_{30}H_{63}O_3P$: t324
$C_{32}H_{64}O_4Sn$: d178
$C_{32}H_{66}$: d823
$C_{36}H_{75}O_3P$: d726
$C_{39}H_{74}O_6$: g21
$C_{40}H_{82}O_6P_2$: b217
$C_{42}H_{82}O_4S$: d727
$C_{45}H_{86}O_6$: g25
$C_{51}H_{98}O_6$: g24
$C_{55}H_{98}O_6P_2$: i111
$C_{57}H_{104}O_6$: g23

TABLE 1.15 Physical Constants of Organic Compounds

See also the special tables of polymers, rubbers, fats, oils, and waxes.

Names of the compounds in the table starting on p. 1.76 are arranged alphabetically. Usually substitutive nomenclature is employed; exceptions generally involve ethers, sulfides, sulfones, and sulfoxides. Each compound is given a number within its letter classification; thus compound c209 is 3-chlorophenol. Section 1.1, Nomenclature of Organic Compounds, should be consulted to familiarize oneself with present nomenclature systems.

Synonyms or Alternate Names are found at the bottom of each spread in their alphabetical listing; the number following the same refers to the numerical place of this compound in the table. For example, epichlorohydrin, c120, indicates that this compound is found listed under the name 1-chloro-2,3-epoxypropane.

Formulas are presented in semistructural form when no ambiguity is possible. Complicated systems are drawn in complete structural form and located at the bottom of each page and keyed to the number of the entry.

Beilstein Reference. In this column is found the reference to the volume and page numbers of the fourth edition of Beilstein, *Handbuch der Organischen Chemie* (Springer-Verlag, New York, 1918). Thus the entry 9, 202 refers to an entry in volume 9 appearing on page 202. When the volume number has a superscript attached, reference is made to the appropriate supplementary volume. For example, 12^2, 404 indicates that the compound will be found listed in the second supplement to volume 12 on page 404. The earliest Beilstein entry is listed. Supplementary information may be found in the supplements to the basic series; such coordinating references (series number, volume number, and page number of the main edition) along with the system number are found at the top of each *odd-numbered page.* Similarly, a back reference such as H93; E II 64; E III 190 in a volume of Supplementary Series IV means that previous items on this compound are found in the same volume of the

Basic Series on page 93, of Supplementary Series II on page 64, and of Supplementary Series III on page 190. The absence of a back reference implies that the compound involved is described *for the first time* in the series concerned.

Formula Weights are based on the International Atomic Weights of 1993 and are computed to the nearest hundredth when justified. The actual significant figures are given in the atomic weights of the individual elements; see Table 3.2.

Density values are given at room temperature unless otherwise indicated by the superscript figure; thus 0.9711^{112} indicates a density of 0.9711 for the substance at 112°C. A density of 0.899^{16}_{4} indicates a density of 0.899 for the substance at 16°C relative to water at 4°C.

Refractive Index, unless otherwise specified, is given for the sodium line at 589.6 nm. The temperature at which the measurement was made is indicated by the superscript figure; otherwise it is assumed to be room temperature.

Melting Point is recorded in certain cases as 250 d and in some other cases as d 250, the distinction being made in this manner to indicate that the former is a melting point with decomposition at 250°C, while the latter decomposition occurs only at 250°C and higher temperatures. Where a value such as $-2H_2O$, 120 is given, it indicates a loss of 2 moles of water per formula weight of the compound at a temperature of 120°C.

Boiling Point is given at atmospheric pressure (760 mmHg) unless otherwise indicated; thus 82^{15mm} indicates that the boiling point is 82°C when the pressure is 15 mmHg. Also, subl 550 indicates that the compound sublimes at 550°C.

Flash Point is given in degrees Celsius, usually using a closed cup. When the method is known, the acronym appears in parentheses after the value: closed cup (CC), Cleveland closed cup (CCC), open cup (OC), Tag closed cup (TCC), and Tag open cup (TOC). Because values will vary with the specific procedure employed, and many times the method was not stated, the values listed for the flash point should be considered only as indicative. See also Table 5.23, Properties of Combustible Mixtures in Air.

Solubility is given in parts by weight (of the formula weight) per 100 parts by weight of the solvent and at room temperature. Other temperatures are indicated by the superscript. Another way in which solubility is explicitly stated is in weight (in grams) per 100 mL of the solvent. In the case of gases, the solubility is often expressed as $5\ mL^{10}$, which indicates that at 10°C, 5 mL of the gas is soluble in 100 g (or 100 mL, if explicitly stated) of the solvent.

Abbreviations Used in the Table

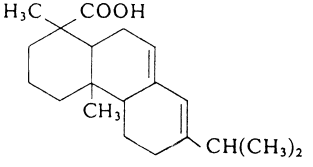
abs, absolute
acet, acetone
alc, alcohol (ethanol usually)
alk, alkali (aqueous NaOH or KOH)
anhyd, anhydrous
aq, aqueous, water
as, asymmetrical
atm, atmosphere
BuOH, 1-butanol
bz, benzene
c, cold
chl, chloroform
conc, concentrated
d, decomposes or decomposed
D, dextrorotatory
deliq, deliquescent
dil, dilute
diox, 1,4-dioxane
DL, inactive (50% **D** and 50% **L**)
DMF, dimethylformamide
E, trans (German "entgegen")
EtOAc, ethyl acetate
eth, diethyl ether
EtOH, ethanol, 95%
expl, explodes
glyc, glycerol
h, hot
HOAc, acetic acid
hyd, hydrolysis
hygr, hygroscopic
i, insoluble
ign, ignites
i-PrOH, isopropyl alcohol, 2-propanol
L, levorotatory
m, meta configuration
Me, methyl
MeOH, methanol
misc, miscible; soluble in all proportions
NaOH, aqueous sodium hydroxide
o, ortho configuration
org, organic
p, para configuration
PE, petroleum ether
pyr, pyridine
s, soluble
sec, secondary
sl, slight, slightly
soln, solution
solv, solvent
subl, sublimes
s, symmetrical
sym, symmetrical
tert, tertiary
v, very
v s, very soluble
v sl s, very slightly soluble
vac, vacuo or vacuum
vols, volumes
Z, cis (German "zusamman")
$>$, greater than
$<$, less than
$\sim$, approximately
$\pm$, inactive [50% (+) and 50% (−)]
α, alpha (first) position
β, beta (second) position
γ, gamma (third) position
δ, delta (fourth) position
ω, omega position (farthest from parent functional group)

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
a1	(−)-Abietic acid		302.46	9^{2}, 424			172–175			i aq; s acet, alc, bz, chl, CS_2, eth, dil alk
a2	Acenaphthene		154.21	5, 586	1.189	1.6048^{95}	93.4	279		i aq; 3.2 alc; 20 bz; 10 chl; 1.8 MeOH; 3.2 g in 100 mL HOAc
a3	Acenaphthylene		152.20	5, 625	0.899_{4}^{16}		88–91	280		i aq; v s alc, eth
a4	Acetaldehyde	CH_3CHO	44.05	1, 594	0.788_{6}^{16}	1.3316^{20}	−123	21	−38(CC)	misc aq, alc, eth
a5	Acetaldoxime	$CH_3CH{=}NOH$	59.07	1, 608	0.966	1.415^{20}	46.5(α) 12(β)	114.5	40	v s aq, alc, eth
a6	Acetamide	CH_3CONH_2	59.07	2^{2}, 177	0.999^{78}	1.4158^{110}	81	222		70 aq; 50 alc; 16 pyr; s chl, glyc, hot bz
a7	Acetamidine HCl	$CH_3C(=NH)NH_2 \cdot HCl$	94.54	2, 185			164–166			v s aq; s alc; i acet, eth
a8	*N*-(2-Acetamido)-2-aminoethanesulfonic acid	$H_2N(CO)CH_2NHCH_2CH_2SO_3H$	182.20				>220 dec			
a9	4-Acetamidobenzaldehyde	$CH_3CONHC_6H_4CHO$	163.18	14, 38			156–158			s aq, bz; sl s alc
a10	4-Acetamidobenzenesulfonyl chloride	$CH_3CONHC_6H_4SO_3Cl$	233.67	14, 702			148 dec			d aq; v s alc, bz, eth, acet
a11	2-Acetamidobenzoic acid	$CH_3CONHC_6H_4CO_2H$	179.18	14, 337			185–187			sl s aq; v s alc, bz, eth, acet
a12	4-Acetamidobenzoic acid	$CH_3CONHC_6H_4CO_2H$	179.18	14, 432			262 dec			i aq; s alc; sl s eth
a13	2-Acetamidofluorene		223.28	12, 1331			192–196			i aq; s alc, glycols
a14	*N*-(2-Acetamido)iminodiacetic acid	$H_2NCOCH_2N(CH_2CO_2H)_2$	190.16				219 d			
a15	2-Acetamidophenol	$CH_3CONHC_6H_4OH$	151.17	13, 370			207–210			
a16	3-Acetamidophenol	$CH_3CONHC_6H_4OH$	151.17	13, 415			146–149			
a17	4-Acetamidophenol	$CH_3CONHC_6H_4OH$	151.17	13, 460	1.293_{4}^{21}		170–172			s alc, acet
a18	Acetanilide	$CH_3CONHC_6H_5$	135.17	12, 237	1.219_{4}^{15}		114	304–305	173	0.56 aq[25]; 25 acet; 29 alc; 2 bz; 27 chl; 5 eth
a19	Acetic acid	CH_3CO_2H	60.05	2, 96	1.0492_{4}^{20}	1.3718^{20}	16.7	118	39 (CC)	misc aq, alc, eth, CCl_4
a20	Acetic acid-*d*	CH_3CO_2D	61.06	2^{3}, 202	1.059	1.2715^{20}		115.5	40	misc aq, alc, eth, CCl_4

a21	Acetic-d_3 acid-d	CD_3CO_2D	64.08	2^3, 203	1.137	1.3687^{20}		114.4	40	misc aq, alc, eth, CCl_4
a22	Acetic anhydride	$(CH_3CO)_2O$	102.09	2, 166	1.080^{15}_4	1.3904^{20}	−73	139	54 (CC)	s chl, eth; slowly s aq forming HOAc, alc forming EtOAc
a23	Acetic anhydride-d_6	$(CD_3CO)_2O$	108.14			1.3875^{20}		65^{65mm}	54	see acetic anhydride
a24	Acetoacetanilide	$CH_3COCH_2CONHC_6H_5$	177.20	12, 518	1.260^{20}		85	dec	185	s alc, hot bz, acids, alkalis, chl, eth
a25	Acetoacetic acid	CH_3COCH_2COOH	102.09	3, 630			36–37	d viol 100		misc aq, alc
a26	Acetone	CH_3COCH_3	58.08	1, 635	0.7908^{20}_4	1.3591^{20}	−94	56	−20	misc aq, alc, chl, DMF
a27	Acetone-d_6	CD_3COCD_3	64.13		0.872	1.3554^{20}	−93.8	55.5	−17	see acetone
a28	Acetone oxime	$(CH_3)_2C{=}NOH$	73.10	1, 649	0.911^{62}_2		60	135		v s aq, alc, eth
a29	Acetonitrile	CH_3CN	41.05	2, 183	0.7875^{15}_4	1.3460^{15}	−44	81.6	6	misc aq, acet, alc, chl, eth, EtOAc
a30	Acetonitrile-d_3	CD_3CN	44.08	2^4, 428	0.844	1.3406^{20}		80.7	5	misc aq, alc, chl
a31	Acetophenone	$C_6H_5COCH_3$	120.15	7, 271	1.026^{20}_4	1.5372^{20}	20	202	77	0.55 aq; s alc, chl, eth, glyc
a32	Acetophenone-methyl-d_3	$C_6H_5COCD_3$	123.18	7^4, 626	1.055	1.5325^{20}		201–202	82	

ACES, a8
Acetal, d303
Acetaldehyde ammonia, a162
Acetaldehyde diethyl acetal, d303
Acetaldehyde dimethyl acetal, d504
Acetamidoacetic acid, a46
2-Acetamidopentanedioic acid, a45
Acetoacetic ester, e58
Acetoin, h108
Acetonaphthones, m322, m323
Acetonecarboxylic acid, a24
Acetone cyanohydrin, h138a
Acetone dimethyl acetal, d519
Acetone ketal of glycerin, d599
Acetonylacetone, h60



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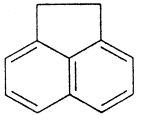
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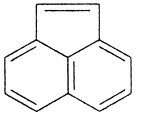
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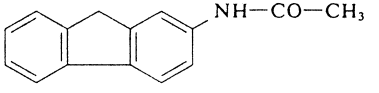


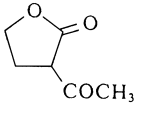
a13

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
a33	4-Acetylbenzenesulfonic acid, sodium salt	$CH_3COC_6H_5SO_3^-\ Na^+$	222.20	11^2, 186			>300			
a34	Acetylbiphenyl	$C_6H_5C_6H_4COCH_3$	196.25	7^2, 337			116–118	325–327		i aq; v s alc, acet
a35	Acetyl bromide	CH_3COBr	122.95	2, 174	1.663_4^{16}	1.4486^{20}	−96	76	>110	dec viol by aq or alc; misc bz, chl, eth
a36	2-Acetylbutyrolactone		128.13	17^3, 5837	1.1846_4^{20}	1.4585^{20}		107^{5mm}	>110	20% v/v aq
a37	Acetyl chloride	CH_3COCl	78.50	2, 173	1.104_4^{20}	1.3896^{20}	−113	51	4 (CC)	dec viol aq or alc; misc bz, chl, eth, HOAc, PE
a38	Acetylcholine bromide	$(CH_3)_3N(Br)CH_2CH_2O_2CCH_3$	226.11	4^1, 428			144–146			v s aq (dec by hot aq or alkalis); s alc; i eth
a39	Acetylcholine chloride	$(CH_3)_3N(Cl)CH_2CH_2O_2CCH_3$	181.66	4, 281			150–152			v s aq, alc; dec by hot aq or alkalis; i eth
a40	2-Acetylcyclopentanone		126.16	7, 558	1.043	1.4905^{20}		75^{8mm}	72	
a41	Acetylene	$HC{\equiv}CH$	26.04	1, 228	0.90(*g*)		−85(subl)		−18	1 vol in 1 vol aq, in 6 vol HOAc or alc; s bz, eth; acet dissolves 25 vol[15] but 300 vols at 12 atm
a42	Acetylenedicarboxylic acid	$HO_2CC{\equiv}CCO_2H$	114.06	2, 801			180 d			v s aq, alc, eth
a43	Acetyl fluoride	CH_3OF	62.04	2, 172	1.002_4^{15}		<−60	20.8		5 aq(dec); sl s acet, alc, bz, eth
a44	2-Acetylfuran		110.11	17, 286	1.098	1.5065^{20}	29–30	67^{10mm}	71	
a45	*N*-Acetyl-(−)-glutamic acid	$HO_2CCH_2CH_2CHCO_2CH_3$ (NHCOCH$_3$)	189.17	4^2, 908			200–201			
a46	*N*-Acetylglycine	$CH_3CONHCH_2CO_2H$	117.10	4, 354			206–208			2.7 aq[15]; s alc; sl s acet, chl, HOAc; i bz, eth
a47	1-Acetylimidazole		110.12				103–105			

a48	Acetyl iodide	CH_3COI	169.95	2, 174	2.0674_4^{20}	1.5491^{20}		108		dec aq, alc; s bz, eth
a49	Acetyl-2-methylcholine chloride	$CH_3CO_2CH(CH_3)CH_2N(Br)(CH_3)_3$	195.69	Merck: 12, 6003			172–173			v s aq, alc, chl; i eth; dec by alkalis, eth
a50	2-Acetylphenothiazine		241.31				180–185			
a51	2-Acetylphenylacetonitrile	$C_6H_5CH(CN)COCH_3$	159.19	10, 699				92–94		
a52	1-Acetyl-4-pipidone		141.17		1.146	1.5026^{20}		218	>110	
a53	2-Acetylpyridine	$(C_5H_4N)COCH_3$	121.14	21, 279	1.080	1.5203^{20}		188–189	73	v s alc, eth
a54	3-Acetylpyridine	$(C_5H_4N)COCH_3$	121.14	21, 279	1.102	1.5336^{20}		220	150	v s acids, alc, eth; s aq
a55	4-Acetylpyridine	$(C_5H_4N)COCH_3$	121.14	21, 279	1.095	1.5350^{20}		212	>110	v s alc, eth
a56	Acetylsalicylic acid	$HO_2C_6H_4$-2-O_2CCH_3	180.16	10, 67	1.35		135			0.33 aq^{25}; 29 acet; 20 alc; 5.9 chl; 5 eth; s bz
a57	2-Acetylthiophene	$(C_4H_3S)COCH_3$	126.18	17, 287	1.168_4^{22}	1.5564^{20}	10–11	214		sl s aq; misc alc, eth
a58	1-Acetyl-2-thiourea	$CH_3C(O)NHC(S)NH_2$	118.16	3, 191			167			s hot aq, alc; sl s eth

p-Acetotoluide, m374
Acetoxime, a28
2-Acetoxybenzoic acid, a56
1-Acetoxy-1,3-butadiene, b378
(Acetoxymethyl)benzene, b76
3-Acetoxypropene, a74
Aceturic acid, a46
Acetylacetanilid, a24
Acetyl acetate, a22
Acetylacetone, p34
N-Acetylanthranilic acid, a11
Acetylbenzene, a31
Acetylcyclopropane, c410
Acetylene dichloride, d228, d229
Acetylene tetrabromide, t16
Acetylene tetrachloride, t37
N-Acetylethanolamine, h119
3-Acetyl-6-methyl-2*H*-pyran-2,4-(3*H*)-dione, d25
2-(Acetyloxy)benzoic acid, a56
3-Acetyl-1-propanol, h164
N-Acetylsulfanilyl chloride, a10



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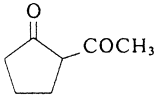

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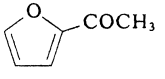

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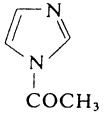

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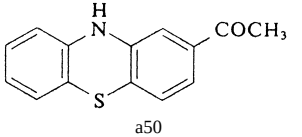

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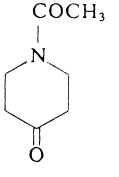


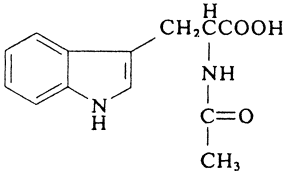
a52

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
a59	*N*-Acetyl-(±)-trypto-phan		246.27	22^{2}, 469			206			s aq, alc; v s eth
a60	Acridine		179.22	20, 459	1.005_{4}^{20}		106–110 subl 100	346		s alc, eth, CS_2, PE; sl s hot aq
a61	Acrylamide	$H_2C{=}CHCONH_2$	71.08	2, 400	1.222_{4}^{30}		84.5	192.6		at 30°, g/100 mL: 215 aq, 155 MeOH, 86 EtOH, 63 acet, 12.6 EtOAc, 2.7 chl, 0.3 bz
a62	Acrylic acid	$H_2C{=}CHCO_2H$	72.06	2, 397	1.0511^{20}	1.4224^{20}	12–14	141	50	misc aq, alc, bz, eth, chl, acet
a63	Acrylonitrile	$H_2C{=}CHCN$	53.06	2, 400	0.8060_{4}^{20}	1.3911^{20}	−83.5	77.3	0	7.3 aq; misc org solv
a63a	Acryloyl chloride	$H_2C{=}CHCOCl$	90.51	2, 400	1.114	1.4350^{20}		72–76	15	d aq; v s chl
a64	1-Adamantanamine		151.25	Merck: 12, 389			160–190			sl s aq
a65	Adamantane		136.24	Merck: 12, 149	1.09	1.568	270 (sealed tube)	205 subl		s acet
a66	Adenine		135.13	26, 420			360 dec	subl 220		0.005 aq; sl s alc; i chl, eth
a67	(−)-Adenosine		267.24	31, 27			235			s aq; i alc
a68	(±)-α-Alanine	$CH_3CH(NH_2)CO_2H$	89.09	4, 387	1.424		264–269 (de-pends on heat-ing rate)	subl >200		16.7 aq^{25}; 0.009 alc^{25}; i eth
a69	(−)-α-Alanine	$CH_3CH(NH_2)CO_2H$	89.09	4, 381	1.401		dec 297			16.7 aq^{25}; 0.2 alc^{25}; i eth
a70	β-Alanine	$H_2NCH_2CH_2CO_2H$	89.09	4, 401	1.437^{-5}		197 dec			v s aq; sl s alc; i eth
a71	Allantoin		158.12	25, 474			238			0.45 aq; 0.2 alc; i eth
a72	Allene	$H_2C{=}C{=}CH_2$	40.06	1, 248	1.787	1.4168	−136	−34		
a73	Alloxan monohydrate		160.09	24, 500			anhyd: 256 dec			s aq, alc, acet, HOAc; sl s chl, EtOAc, PE
a74	Allyl acetate	$H_2C{=}CHCH_2OCOCH_3$	100.12	2, 136	0.977_{4}^{20}	1.4040^{20}		104	22	i aq; misc alc, eth
a75	Allyl alcohol	$H_2C{=}CHCH_2OH$	58.08	2, 436	0.8540_{4}^{20}	1.4134^{20}	−129	97	21	misc aq, alc, chl, eth
a76	Allylamine	$H_2C{=}CHCH_2NH_2$	57.10	4, 205	0.761_{4}^{20}	1.4185^{20}	−88.2	53–55	−29	misc aq, alc, chl, eth

a77	*N*-Allylaniline	$C_6H_5NHCH_2CH{=}CH_2$	133.19	12, 170	0.982^{25}	1.5630^{20}		220	89	i aq; s alc, eth
a78	Allylbenzene	$C_6H_5CH_2CH{=}CH_2$	118.18	5, 484	0.892_0^{20}	1.5122^{20}		157	33	i aq; s alc, eth
a79	Allyl bromide	$H_2C{=}CHCH_2Br$	120.98	1, 201	1.398_4^{20}	1.4654^{20}	−119	70	−2	sl s aq; misc org solv
a80	Allyl butanoate	$CH_3CH_2CH_2COOCH_2$-$CH{=}CH_2$	128.17	2, 272	0.902	1.4142^{20}	44^{15mm}	41		

Aconitic acid, p206
Acrolein, p203
Acrolein diethyl acetal, d312
Acrolein dimethyl acetal, d521
Acrylaldehyde, p203
Adipic acid, h54
Adipic acid monoethyl ester, e177
Adiponitrile, d284
Alaninol, a264, a265
Allocimene, d669
Allylacetone, h77
4-Allylanisole, a89
Allyl butyrate, a80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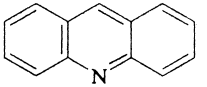
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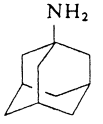
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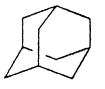
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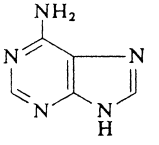
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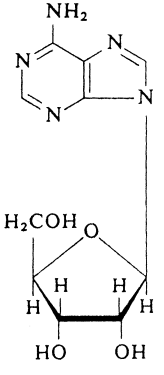
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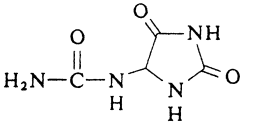
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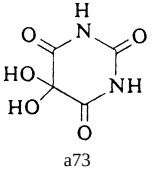
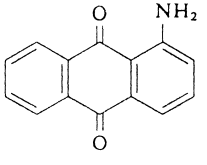

a73

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
a81	Allyl chloride	$H_2C{=}CHCH_2Cl$	76.53	1, 198	0.938_4^{20}	1.4154^{20}	−134.5	44–46	−31 (CC)	sl s aq; misc alc, chl, eth, PE
a82	Allyl chloroformate	$H_2C{=}CHCH_2OOCCl$	120.54	3, 12	1.136	1.4223	110	27	31	
a83	Allylcyclohexylamine	$(C_6H_{11})NHCH_2CH{=}CH_2$	139.24		0.962	1.4664^{20}		66^{12mm}	53	
a84	4-Allyl-1,2-dimethoxybenzene	$H_2C{=}CHCH_2C_6H_3(OCH_3)_2$	178.23	6, 963	1.036	1.5344^{20}	−4	255		
a85	*N*-Allyl-*N*,*N*-dimethylamine	$H_2C{=}CHCH_2N(CH_3)_2$	85.0			1.4010^{20}		64		
a86	Allyl ethyl ether	$H_2C{=}CHCH_2OCH_2CH_3$	86.13	1, 438	0.765_4^{20}	1.3881^{20}		68	−20	i aq; misc alc, eth
a87	Allyl iodide	$H_2C{=}CHCH_2I$	167.98	1, 202	1.825_4^{20}	$1,5540^{21}$	−99	103		i aq; misc alc, eth
a88	Allyl isothiocyanate	$H_2C{=}CHCH_2NCS$	99.16	4, 214	1.013_4^{25}	1.5248^{25}	−80	152	46	0.2 aq; misc org solv
a89	Allyl methacrylate	$H_2C{=}C(CH_3)COOCH_2$-$CH{=}CH_2$	126.16	2^3, 1290	0.938	1.4360		61^{43mm}	33	
a90	Allyl methyl sulfide	$H_2C{=}CHCH_2SCH_3$	88.17	1, 440	0.803	1.4714^{20}		91–93	18	
a91	1-Alloxy-2,3-epoxypropane	$H_2C\!-\!CHCH_2OCH_2$- $\backslash\ /$ $O\quad CH{=}CH_2$	114.14		0.962	1.4332^{20}		154	57	
a92	3-Alloxy-1,2-propanediol	$H_2C{=}CHCH_2$- $CH_2CH(OH)CH_2OH$	132.16	1, 513	1.068	1.4620^{20}		142^{28mm}	>110	
a93	Alloxytrimethylsilane	$H_2C{=}CHCH_2OSi(CH_3)_3$	130.26		0.7830	1.4075^{25}		102	0	
a94	2-Allylphenol	$H_2C{=}CHCH_2C_6H_4OH$	134.18	6, 572	1.033_4^{15}	1.5450^{20}	10	220	88	s alc, eth
a95	Allyl phenyl ether	$H_2C{=}CHCH_2OC_6H_5$	134.18	6, 144	0.983_4^{15}	1.5200^{20}		192	62	i aq; s alc, misc eth
a96	Allyl propyl ether	$H_2C{=}CHCH_2OC_3H_7$	100.16	1, 438	0.767_4^{20}	1.3990^{20}		90–92	−5	s alc; misc eth
a97	1-Allyl-2-thiourea	$H_2C{=}CHCH_2NHC(S)NH_2$	116.19	4, 211	1.219_{20}^{20}		70–72			3.3 aq; s alc; i bz; v sl s eth
a98	Allyltrichlorosilane	$H_2C{=}CHCH_2SiCl_3$	175.52	4^3, 1909	1.2011_4^{20}	1.4550^{20}		117.5	31	
a99	Allyltriethoxysilane	$H_2C{=}CHCH_2Si(OC_2H_5)_3$	204.34	4^3, 1909	0.9030^{20}	1.4062^{20}		176^{740mm}	21	
a100	Allyl trifluoroacetate	$CF_3COOCH_2CH{=}CH_2$	154.09	2^4, 464	1.183	1.3350^{20}		66–67	−1	
a101	Allyltrimethylsilane	$H_2C{=}CHCH_2Si(CH_3)_3$	114.27		0.7193_4^{20}	1.4080^{20}		84–88	7	
a102	Allylurea	$H_2C{=}CHCH_2NHCONH_2$	100.12	4, 209			85			v s aq, alc; i chl, CS_2 eth, toluene
a103	Aminoacetonitrile	H_2NCH_2CN	56.07	4, 344				58^{15mm} d		s acids, alc

a104	Aminoacetonitrile hydrogen sulfate	$H_2NCH_2CN \cdot H_2SO_4$	154.14	4, 344			121	d 165		v s aq; sl s alc; i eth
a105	2′-Aminoacetophenone	$H_2NC_6H_4COCH_3$	135.17	14, 41				70^{3mm}	>110	v sl s aq; s alc, eth
a106	3′-Aminoacetophenone	$H_2NC_6H_4COCH_3$	135.17	14, 45			99	290		
a107	4′Aminoacetophenone	$H_2NC_6H_4COCH_3$	135.17	14, 46			106	293–295		s hot aq, alc, eth, HOAc; sl s bz
a108	1-Aminoanthraquinone		223.23	14, 177			ca. 250	subl		i aq; v s alc, bz, chl, eth, HOAc, HCl
a109	2-Aminoanthraquinone		223.23	14, 191			295 d	subl		i aq, eth; s alc, bz
a110	4-Aminoantipyrine		203.25	24, 273			109			s aq, alc, bz; sl s eth
a111	*p*-Aminoazobenzene	$C_6H_5N{=}NC_6H_4NH_2$	197.24				128	>360		sl a aq; v s alc, bz, chl, eth
a112	2-Aminobenzamide	$H_2NC_6H_4CONH_2$	136.15	14, 320			110	300 sl d		v s hot aq, alc; i bz; sl s eth
a113	4-Aminobenzenearsonic acid	$H_2NC_6H_4AsO(OH)_2$	217.06	16, 878			232			s hot aq; alk CO_3, conc′d mineral acids; i acet, bz, chl, eth
a114	5-Aminobenzene-1,3-dicarboxylic acid	$H_2NC_6H_3(COOH)_2$	181.15	14[1], 636			>300			

Allyl carbamide, a102
Allyl chloride, c236a
Allyl cyanide, b482
Allyl glycidyl ether, a91
1-Allyl-2-hydroxybenzene, a94
Allyl iodide, i50
Allyl mercaptan, p205
Allyl sulfide, d34
Allyl trichloride, t247
Aluminon, a306
N-Amidinosarcosine, c301
Aminoacetaldehyde diethyl acetal, d306
Aminoacetaldehyde dimethyl acetal, d506
1-Aminoadamantane, a64
Aminoanisoles, m48 thru m50
p-Aminoazobenzene, p88



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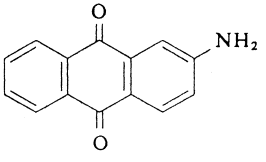

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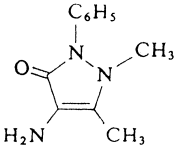

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TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
a115	2-Aminobenzene-sulfonic acid	$H_2NC_6H_4SO_3H$	173.19	14, 681			ca. d 325			1.5 aq[15]; v sl s alc, eth
a116	3-Aminobenzene-sulfonic acid	$H_2NC_6H_4SO_3H$	173.19	14, 688	1.69		>300			2 aq[15]; sl s alc, MeOH
a117	4-Aminobenzene-sulfonic acid	$H_2NC_6H_4SO_3H$	173.19	14, 695			d 288			1 aq[20]; sl s hot MeOH; i alc, bz, eth
a118	2-Aminobenzoic acid	$H_2NC_6H_4COOH$	137.14	14, 310			144–146	subl		v s hot aq, alc, eth
a119	3-Aminobenzoic acid	$H_2NC_6H_4COOH$	137.14	14, 383	1.511^{4}		172–174			v s hot aq, alc; s eth
a120	4-Aminobenzoic acid	$H_2NC_6H_4COOH$	137.14	14, 418	1.374		187			0.59 aq; 12 alc; 2 eth; s EtOAc, HOAc
a121	2-Aminobenzonitrile	$H_2NC_6H_4CN$	118.14	14, 322			49	268	>110	s alc, eth
a122	3-Aminobenzonitrile	$H_2NC_6H_4CN$	118.14	14, 391			53	288–290	>110	s hot aq; v s alc, eth
a123	4-Aminobenzonitrile	$H_2BC_6H_4CN$	118.14	14, 425			85	dec		v s hot aq, alc, eth
a124	2-Aminobenzophenone	$H_2NC_6H_4COC_6H_5$	197.24	14, 76			108	223–226		sl s aq; s alc, eth
a125	2-Aminobenzothiazole		150.20	27, 182			132	dec		v s conc′d acids, alc, chl, eth
a126	2-Aminobenzotri-fluoride	$H_2NC_6H_4CF_3$	161.13	12^{12}, 453	1.290^{25}	1.4785^{25}	34	175	55	
a127	3-Aminobenzotri-fluoride	$H_2NC_6H_4CF_3$	161.13	12, 870	1.290	1.4800^{20}	6	187	85	
a128	4-Aminobenzotri-fluoride	$H_2NC_6H_4CF_3$	161.13	12^{3}, 2151	1.283^{27}	1.4815^{25}	38	83^{12mm}	86	
a129	*N*-(4-Aminobenzoyl)-glycine	$H_2NC_6H_4CONHCH_2COOH$	194.19	14^{2}, 258			198–199			i aq; s alc, bz, chi
a130	2-Aminobiphenyl	$H_2NC_6H_4C_6H_5$	169.23	12, 1317			50–53	299	>110	sl s aq; s alc
a131	4-Aminobiphenyl	$H_2NC_6H_4C_6H_5$	169.23	12, 1318			52–54	191^{15mm}	>110	s hot aq, alc, eth
a132	2-Amino-5-bromo-benzoic acid	$Br(NH_2)C_6H_3COOH$	216.03	14, 370			218–219			s alc, bz, chl, eth, HOAc; v s acet
a133	(±)-2-Aminobutanoic acid	$CH_3CH_2CH(NH_2)COOH$	103.12	4, 408			304 d	subl >300		21 aq[25], 0.18 hot alc; i eth
a133a	3-Aminobutanoic acid	$H_3CCH_2CH(NH_2)COOH$	103.12	4, 412			193–194			125 aq; i alc, eth
a134	4-Aminobutanoic acid	$H_2NCH_2CH_2CH_2COOH$	103.12	4, 413			195 d			v s aq; i org solv
a135	2-Amino-1-butanol	$CH_2CH_2CH(NH_2)CH_2OH$	89.14	4, 291	0.944^{20}_{20}	1.4521^{20}	−2	176–178	74 (OC)	misc aq; s alc

a136	3-(4-Aminobutyl)-piperidine	$(HNC_5H_9)(CH_2)_4NH_2$	156.27	22[3], 3788	0.910		39–42	148[10mm]	>110	
a137	4-Amino-6-chloro-1,3-benzenedisulfonamide	$H_2NC_6H_2(Cl)(SO_2NH_2)_2$	285.73	14[4], 2810			257–261			
a138	2-Amino-4-chlorobenzoic acid	$H_2N(Cl)C_6H_3COOH$	171.58	14, 365			231–233			
a139	5-Amino-2-chlorobenzoic acid	$H_2N(Cl)C_6H_3COOH$	171.58	14, 412			188 d			
a140	2-Amino-4′-chlorobenzophenone	$H_2NC_6H_4COC_6H_4Cl$	231.68	14[1], 389			104			
a141	2-Amino-5-chlorobenzophenone	$H_2N(Cl)C_6H_3COC_6H_5$	231.68	14, 79			98–100			
a142	2-Amino-5-chlorobenzotrifluoride	$H_2N(Cl)C_6H_3CF_3$	195.57	12[3], 1921	1.386	1.5069^{20}		67[3mm]	none	
a143	5-Amino-2-chlorobenzotrifluoride	$H_2N(Cl)C_6H_3CF_3$	195.57				36–38		>110	
a144	2-(3-Amino-4-chlorobenzoyl)benzoic acid	$H_2N(Cl)C_6H_3COC_6H_4COOH$	275.69	14, 661			171–173			
a145	4-Amino-4′-chlorobiphenyl	$H_2NC_6H_4$–C_6H_4Cl	203.67				128–134			i aq; s alc, acet, bz, chl, HOAc
a146	4-Amino-5-chloro-2-methoxybenzoic acid	$H_2NC_6H_2(Cl)(OCH_3)COOH$	201.61				206 d			
a147	2-Amino-4-chlorophenol	$H_2N(Cl)C_6H_3OH$	143.57	13, 383			139–143			
a148	2-Amino-5-chloropyridine	$H_2N(Cl)(C_5H_3N)$	129.56	22[2], 332			135–138	128[11mm]		

Aminobenzenethiol, a297
Aminobenzyl cyanide, a255
1-Aminobutane, b509

2-Aminobutane, b510
4-Aminobutyraldehyde diethyl acetal, d299
Aminobutyric acids, a133, a133a, a134

α-Aminocaproic acid, a182
ϵ-Aminocaproic acid, a183

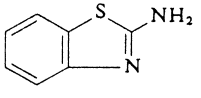

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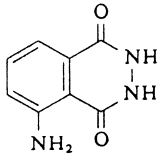
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
a149	3-Aminocrotononitrile	$CH_3C(NH_2)=CHCN$	82.11	3, 660						
a150	1-[(2-Aminoethyl)-amino]-2-propanol	$CH_3CH(OH)CH_2NHCH_2CH_2NH_2$	118.18		0.9837_4^{25}	1.4788^{25}		112^{10mm}		
a151	5-Amino-2,3-dihydro-1,4-phthalazinedione		177.16	25[1], 698			319–320			
a152	2-Amino-4,6-dihy-droxypyrimidine		127.10	24, 468			>300			
a153	4-Amino-2,6-dihy-droxypyrimidine		127.10	24, 469			>300			
a154	2-Amino-3,3-dimethyl-butane	$(CH_3)_3CCH(NH_2)CH_3$	101.19	4, 193	0.755	1.4130^{20}	−20	102–103	1	
a155	2-Amino-4,6-dimethyl-pyridine	$(CH_3)_2(NH_2)(C_5H_2N)$	122.17	22, 435			63–64	235		
a156	4-Amino-2,6-dimethyl-pyrimidine		123.16	24[2], 45			184–186			156 aq; 18.9 alc
a157	6-Amino-1,3-dimethyl-uracil		155.16	24, 471			295 d			
a158	5-Amino-2,6-dioxo-1,2,3,6-tetrahydro-4-pyrimidinecarbox-ylic acid		171.11	25, 264			>300			
a159	α-Aminodiphenyl-methane	$(C_6H_5)_2CHNH_2$	183.25	12, 1323	1.0635_4^{22}	1.5950^{20}	34	304	>110	sl s aq; s acids
a160	2-Aminoethanesulfonic acid	$H_2NCH_2CH_2SO_3H$	125.15	4, 528			d ca. 300			5.45 aq[12]; 0.004 alc[17]
a161	2-Aminoethanethiol	$HSCH_2CH_2NH_2$	77.14	4, 286			97–99			v s aq; s alc
a162	1-Aminoethanol	$CH_2CH(OH)NH_2$	61.08				97	110 d		s aq; sl s eth
a163	2-Aminoethanol	$H_2NCH_2CH_2OH$	61.08	4, 274	1.0117_4^{25}	1.4539^{20}	10.3	171	93	misc aq, org solv
a164	2-(2-Aminoethoxy)-ethanol	$H_2NCH_2CH_2OCH_2CH_2OH$	105.14	4[3], 642	1.048			218–224		
a165	2-(2-Aminoethyl-amino)ethanol	$H_2NCH_2CH_2NHCH_2CH_2OH$	104.15	4, 286	1.030	1.4861^{20}		240^{753mm}	>110	v s aq, alc; sl s eth
a166	1-[(2-Aminoethyl)-amino]-2-propanol	$CH_3CH(OH)CH_2NHCH_2CH_2NH_2$	118.18	Merck: 12, 458	0.9837_4^{25}	1.4738^{25}		112^{10mm}		s acids

a167	3-(2-Aminoethyl-amino)propyltri-methoxysilane	$H_2NCH_2CH_2NHCH_2CH_2$-$Si(OCH_3)_3$	222.1		1.01_4^{25}	1.4418^{25}		140^{15mm}	150	
a168	3-Amino-9-ethylcarba-zole		210.28	22^1, 642			98–100			
a169	2-Aminoethyl hydro-gen sulfate	$H_2NCH_2CH_2OSO_3H$	141.15	4, 276			277 d			
a170	3-(2-Aminoethyl)-indole		160.22	22^1, 636			118	$137^{0.15mm}$		i aq, bz, chl, eth; s alc, acet, HCl
a171	S-2-Aminoethyliso-thiouronium bro-mide HBr		281.01	Merck: 12, 176			194–195			
a172	*N*-(2-Aminoethyl)-morpholine		130.19	27^3, 370	0.992	1.4755^{20}	25.6	205	175	s aq, alc, bz, acet, acids

4-Amino-*m*-cresol, a213
Aminocyclododecane, c340
Aminocyclohexane, c375
Aminodecane, d23
2-Amino-5-diethylaminopentane, d387
2-Amino-1,5-dihydro-1-methyl-4*H*-imidazol-4-one, c302
2-Aminodiphenylamine, p137
Aminodiphenylmethane, d761
Aminoethane, e63
2-Aminoethanol, e29
1-(2-Aminoethyl)amino-2-[(2-aminoethyl)aminoethyl]aminoethane, t56
Aminoethylbenzene, e69, e70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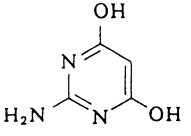
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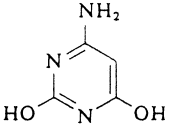
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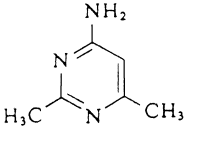
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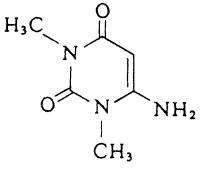
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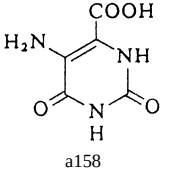
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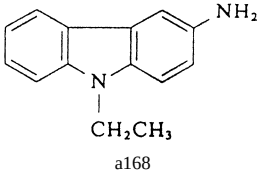
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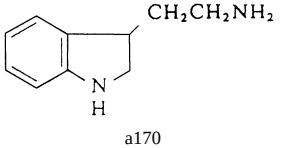
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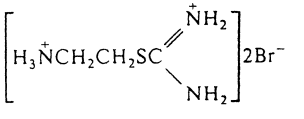
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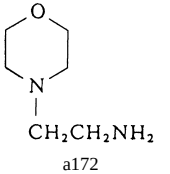
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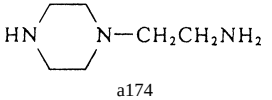
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
a173	4-(2-Aminoethyl)-phenol	$HOC_6H_4CH_2CH_2NH_2$	137.18	13, 625			164–165	166^{2mm}		1 aq[15]; 10 boiling alc; s HCl
a174	*N*-(2-Aminoethyl)-piperazine		129.21		0.985^{20}_{20}	1.4983^{20}	−26	218–222	93 (OC)	
a175	*N*-(2-Aminoethyl)-1,3-propanediamine	$H_2NCH_2CH_2CH_2NHCH_2CH_2NH_2$	117.20		0.928	1.4815^{20}			96	
a176	2-Amino-2-ethyl-1,3-propanediol	$HOCH_2C(NH_2)(C_2H_5)CH_2OH$	119.16	4,3,850	1.099^{20}_{20}	1.490^{20}	38	152^{10mm}	>110	misc aq; s alc
a177	2-(2-Aminoethyl)-pyridine	$H_2NCH_2CH_2(C_5H_4N)$	122.17	22, 434	1.021	1.5360^{20}		93^{12mm}	100	
a178	4-(2-Aminoethyl)-pyridine	$H_2NCH_2CH_2(C_5H_4N)$	122.17		1.012	1.5403^{20}		104^{9mm}		
a179	2-Amino-5-fluorobenzotrifluoride	$H_2N(F)C_6H_3CF_3$	179.12	12^3, 1991	1.3781	1.4608^{20}		81^{20mm}	70	
a180	Aminoguanidine hydrogen carbonate	$H_2NNHC(=NH)NH_2 \cdot H_2CO_3$	136.11	3, 117			172 d			i aq; d hot aq
a181	*N*-Aminohexamethyleneimine	$(C_6H_{12}N)NH_2$	114.19		0.984	1.4850^{20}		165	56	
a182	(±)-2-Aminohexanoic acid	$CH_3(CH_2)_3CH(NH_2)COOH$	131.17	4, 433	1.172		301			1.15 aq[25]; 0.42 alc[25]; s acids
a183	6-Aminohexanoic acid	$H_2N(CH_2)_5COOH$	131.17	4, 434			204–206			v s aq; i alc, s acids
a184	6-Amino-1-hexanol	$H_2N(CH_2)_5CH_2OH$	117.19	4^2, 748			56–58	135^{30mm}		
a185	(−)-2-Amino-3-hydroxybutanoic acid	$CH_3CH(OH)CH(NH_2)COOH$	119.12	4, 514			d 255			v s aq; i alc, chl, eth
a186	(±)-4-Amino-3-hydroxybutanoic acid	$H_2NCH_2CH(OH)CH_2COOH$	119.12	4^2, 938			218 d			s aq; sl s alc, chl, eth, EtOAc
a187	4-Amino-6-hydroxy-2-mercaptopyrimidine hydrate		161.18	24, 476			>300			
a188	2-Amino-4-hydroxy-6-methylpyrimidine		125.13	24, 343			>300			
a189	4-Amino-3-hydroxy-1-naphthalenesulfonic acid		239.25	14, 846			295 d			i aq, alc, bz, eth

a190	4-Amino-5-hydroxy-1-naphthalenesulfonic acid		239.25	14, 835						sl s aq; i alc, eth
a191	5-Amino-6-hydroxy-2-naphthalenesulfonic acid		239.25							sl s hot aq; i eth
a192	6-Amino-7-hydroxy-2-naphthalenesulfonic acid		239.25	14, 849			>300			
a193	2-Amino-3-hydroxy-pyridine	$H_2N(HO)(C_5H_3N)$	110.12	12^{2}, 408			172–174			
a194	4-Amino-2-hydroxy-pyrimidine		111.10	24, 314			>300			0.77 aq; sl s alc
a195	1-Aminoindane		133.19	12, 1191	1.038_4^{15}	1.5613^{20}	1.5	97^{8mm}	94	sl s aq
a196	5-Aminoindane		133.19	12^{1}, 511			36	249^{745mm}	>110	sl s aq

2-(2-Aminoethyl)-2-thiopseudourea, a171
1-Aminoheptane, h19
2-Aminoheptane, m272
1-Aminohexane, h81
2-Aminohexane, m371
p-Aminohippuric acid, a129
Aminohydroxybenzoic acids, a280, a281
2-Amino-2-(hydroxymethyl)-1,3-propanediol, t439
α-Amino-4-imidazolepropanoic acid, h83
Aminoiminomethanesulfinic acid, f34
N-(Aminoiminomethyl)-*N*-methylglycine, c301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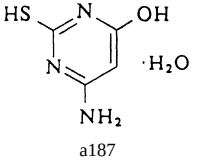
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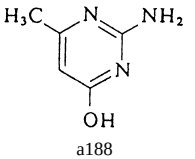
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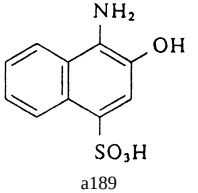
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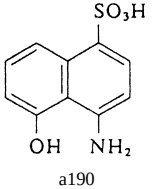
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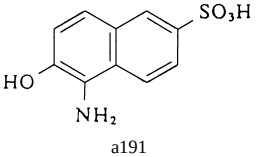
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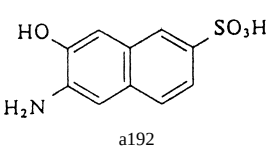
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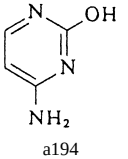
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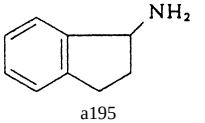
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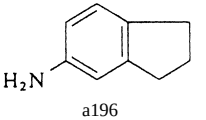
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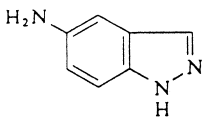
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
a197	5-Aminoindazole		133.15	25[2], 308			175–178			
a198	6-Aminoindazole		133.15	25, 317			206 d			
a199	2-Amino-5-iodobenzoic acid	$H_2N(I)C_6H_3COOH$	263.03	14, 373			221 d			sl s aq, PE; s alc
a200	(±)-2-Amino-4-mercaptobutanoic acid	$HSCH_2CH_2CH(NH_2)COOH$	135.19	4[3], 1647			232–233			
a201	Aminomethanesulfonic acid	$H_2NCH_2SO_3H$	111.12	1, 583			185 d			v s aq
a202	3-Amino-4-methoxybenzoic acid	$CH_3O(NH_2)C_6H_3COOH$	167.16	14[1], 657			210			
a203	2-Amino-1-methoxypropane	$CH_3OCH_2CH(CH_3)NH_2$	84.14	4[4], 1615	0.845	1.4065^{20}		93	8	
a204	5-Amino-2-methoxypyridine	$CH_3O(NH_2)(C_5H_3N)$	124.14	22[2], 408		1.5745^{20}	31	90^{1mm}	>110	
a205	4′-Amino-*N*-methylacetanilide	$CH_3ON(CH_3)C_6H_4NH_2$	164.21	13[1], 30			90–92			
a206	4-Amino-3-methylbenzenesulfonic acid	$H_2NC_6H_3(CH_3)SO_3H$	187.22	14, 726			>300			
a207	2-Amino-5-methylbenzoic acid	$H_2N(CH_3)C_6H_3COOH$	151.17	14, 481			175 d			sl s aq; s alc, eth
a208	3-Amino-4-methylbenzoic acid	$H_2N(CH_3)C_6H_3COOH$	151.17	14, 487			167–169			s aq
a209	2-Amino-3-methyl-1-butanol	$(CH_3)_2CHCH(NH_2)CH_2OH$	103.17	4[3], 805	0.906	1.4543^{20}	35–36	80^{8mm}	90	
a210	2-(Aminomethyl)-1-ethylpyrrolidine		128.22		0.887	1.4665^{20}		60^{16mm}	60	
a211	2-Amino-3-methyl-1-pentanol	$CH_2CH_2CH(CH_3)CH(NH_2)CH_2OH$	117.19			1.4589^{20}	30	97^{14mm}	100	
a212	2-Amino-4-methyl-1-pentanol	$CH_3CH(CH_3)CH_2CH(NH_2)CH_2OH$	117.19	4, 298	0.917	1.4496^{20}		200	90	
a213	4-Amino-3-methylphenol	$H_2N(CH_3)C_3H_3OH$	123.16				179			
a214	4-(Aminomethyl)-piperidine		114.19			1.4900^{20}	25	200	78	

a215	2-Amino-2-methyl-1,3-propanediol	$HOCH_2C(CH_3)(NH_2)CH_2OH$	105.14				108–110	151^{10mm}		250 aq^{20}; s alc
a216	2-Amino-2-methyl-1-propanol	$(CH_3)_2C(NH_2)CH_2OH$	89.14	4^3, 783	0.934^{20}_{20}	1.4480^{20}	25	165	67	misc aq; s alc, org solv
a217	2-Amino-2-methyl-propionic acid	$(CH_3)_2C(NH_2)COOH$	103.12	4, 414			335 (sealed tube)	280 subl		v s aq
a218	2-(Aminomethyl)-pyridine	$H_2NCH_2(C_5H_4N)$	108.14		1.049	1.5440^{20}		85^{12mm}	90	
a219	3-(Aminomethyl)-pyridine	$H_2NCH_2(C_5H_4N)$	108.14		1.062	1.5510^{20}	−21	74^{1mm}	100	
a220	4-(Aminomethyl)-pyridine	$H_2NCH_2(C_5H_4N)$	108.14	22^3, 4181	1.065	1.5515^{20}	−8	230	108	
a221	2-Amino-3-methyl-pyridine	$H_2N(CH_3)(C_5H_3N)$	108.14	22^2, 342	1.073	1.5823^{20}	32–34	222	111	
a222	2-Amino-4-methyl-pyridine	$H_2N(CH_3)(C_4H_3N)$	108.14	22^2, 342			98–100	230		v s aq, alc, DMF
a223	2-Amino-6-methyl-pyridine	$H_2N(CH_3)(C_4H_3N)$	108.14	22^1, 633			42–45	209	103	v s aq
a224	2-Amino-4-methyl-pyrimidine		109.13	24, 84			160	subl		s hot aq; s alc
a225	2-Amino-4-methyl-thiazole		114.17	27, 159			44–46	232	>110	v s aq, alc, eth

2-Aminoisobutanol, a216
2-Aminoisobutyric acid, a217
5-Aminoisophthalic acid, a114
2-Amino-3-mercaptopropanoic acid, c411
1-Amino-2-methoxyethane, m77
α-(Aminomethyl)benzyl alcohol, a257
3-Amino-α-methylbenzyl alcohol, a256
2-Amino-3-methylpentanoic acid, i88
2-Amino-2-methylpropane, b511



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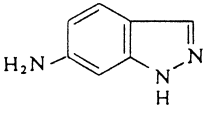

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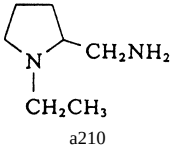

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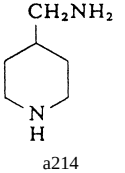

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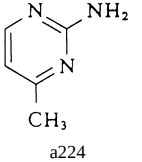

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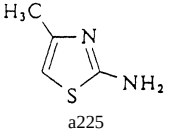

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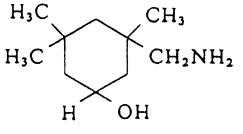
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
a226	2-Aminomethyl-3,5,5-trimethylcyclohexanol		171.29		0.969	1.4904^{20}	43–48	265	>110	
a227	*N*-Aminomorpholine		102.14	27, 8	1.059	1.4772^{20}		168	58	
a228	1-Aminonaphthalene	$(C_{10}H_7)NH_2$	143.18	12, 1212	1.13		48–50	301	157	0.17 aq; v s alc, eth
a229	2-Aminonaphthalene	$(C_{10}H_7)NH_2$	143.18	12, 1212			111–113	306		s hot aq, alc, eth
a230	2-Amino-1-naphthalenesulfonic acid	$H_2N(C_{10}H_6)SO_3H$	223.25	14, 736			dec			0.031 aq; sl s hot aq; s dil alkali
a231	5-Amino-2-naphthalenesulfonic acid	$H_2N(C_{10}H_6)SO_3H$	223.25	14, 758			180			sl s aq; s hot aq
a232	8-Amino-2-naphthol	$H_2NC_{10}H_6OH$	159.19	13, 685			207			
a233	2-Amino-4-nitrobenzoic acid	$H_2N(NO_2)C_6H_3COOH$	182.14	14, 374			270 d			i aq; v s alc, eth
a234	2-Amino-5-nitrobenzonitrile	$H_2N(NO_2)C_6H_3CN$	163.14	14^2, 234			200–207			
a235	5-Amino-5-nitrobenzophenone	$C_6H_5COC_6H_4(NH_2)NO_2$	242.23	14, 79			166–168			
a236	2-Amino-6-nitrobenzothiazole		195.20	27^2, 232			247–249			
a237	4-Amino-3-nitrobenzotrifluoride	$H_2N(NO_2)C_6H_3CF_3$	206.12				105–106			
a238	2-Amino-4-nitrophenol	$O_2N(NH_2)C_6H_3OH$	154.13	13^2, 192			143–145			
a239	2-Amino-5-nitrophenol	$O_2N(NH_2)C_6H_3OH$	154.13	13, 390			202 d			
a240	4-Amino-2-nitrophenol	$O_2N(NH_2)C_6H_3OH$	154.13	13, 520			125–127			
a241	D-(−)-*threo*-2-Amino-1-(4-nitrophenyl)-1,3-propanediol	$HOCH_2C(NH_2)C(OH)C_6H_4NO_2$	212.21				163–165			
a242	2-Amino-5-(4-nitrophenylsulfonyl-thiazole		285.30				222–226			
a243	2-Amino-5-nitropyridine	$H_2N(C_5H_3N)NO_2$	139.11	22^1, 631			186–188			sl s aq, bz, eth
a244	2-Amino-5-nitrothiazole		145.14	Merck: 12, 477			d 202			s sl s aq; 0.7 alc; 0.4 ether; s dil acids

a245	*exo*-2-Aminonor-bornane		111.19	12[3], 160	0.938	1.4807^{20}		49^{10mm}	35	
a246	2-Aminopentane	$H(CH_2)_3CH(NH_2)CH_3$	87.17	4, 177	0.739^{20}	1.4047^{20}		91–92		s aq, alc, eth, PE
a247	3-Aminopentane	$C_2H_5CH(NH_2)C_2H_5$	87.17	4, 179	0.749^{20}_{4}	1.4055^{20}		91	1	misc aq, alc, eth
a248	**DL**-2-Aminopentanoic acid	$H(CH_2)_3CH(NH_2)COOH$	117.15	4, 416			303	320 subl		5.5 aq[18]; v sl s alc, chl, eth, PE
a249	5-Aminopentanoic acid	$H_2N(CH_2)_4COOH$	117.15	4, 418			158–161			v s aq; sl s alc; i eth
a250	5-Amino-1-pentanol	$H_2N(CH_2)_5OH$	103.17	4[1], 441	0.949	1.4615^{20}	35–37	122^{16mm}	65	
a251	2-Aminophenethyl alcohol	$H_2NC_6H_4CH_2CH_2OH$	137.18	13[3], 1679	1.045	1.5849^{20}		148^{4mm}	>112	
a252	2-Aminophenol	$H_2NC_6H_4OH$	109.13	13, 354			170–174			2 aq; 4.3 alc; v s eth
a253	3-Aminophenol	$H_2NC_6H_4OH$	109.13	13, 401			122–123	164^{11mm}		2.5 aq; v s hot aq, alc, eth
a254	4-Aminophenol	$H_2NC_6H_4OH$	109.13	13, 427			190	150^{3mm}		0.65 aq; 4.5 alc; 9.3 EtMeKetone[58]; s eth
a255	4′-Aminophenylacetonitrile	$H_2NC_6H_4CH_2CN$	132.17				45–48	312	>110	sl s hot aq; s alc
a256	1-(3-Aminophenyl)-ethanol	$H_2NC_6H_4CH(CH_3)OH$	137.18	13[3], 1654			68–71			
a257	2-Amino-1-phenyl-ethanol	$H_2NCH_2CH(C_6H_5)OH$	137.18	13[2], 361			56–58	160^{17mm}		v s aq; s alc

1-Aminonaphthalene, n17
1-Amino-2-naphthol-4-sulfonic acid, a189
1-Amino-2-naphthol-6-sulfonic acid, a197
1-Aminoorotic acid, a158
1-Aminopentane, p53



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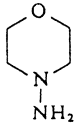

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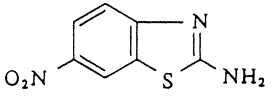

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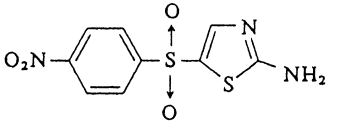

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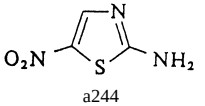

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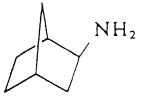

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TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

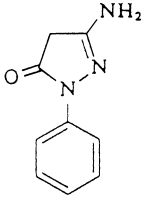
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
a258	1*S*,2*S*-(+)-2-Amino-1-phenyl-1,3-propanediol	$C_6H_5CH(OH)CH(NH_2)CH_2OH$	167.21	13,*4*, 2968			109–113			
a259	**L**-2-Amino-3-phenyl-1-propanol	$C_6H_5CH_2(NH_2)CH_2OH$	151.21	13^3, 1757			92–94			
a260	3-Amino-1-phenyl-2-pyrazolin-5-one		175.19				210 d			
a261	*N*-Aminopiperidine		100.17	20, 89	0.928	1.4750^{20}		146^{730mm}	36	
a262	3-Amino-1,2-propanediol	$H_2NCH_2CH(OH)CH_2OH$	91.11	4, 301	1.175	1.4920^{20}		265^{739mm}	>110	
a263	**DL**-1-Amino-2-propanol	$CH_3CH(OH)CH_2NH_2$	75.11	4, 289	0.973	1.4483^{20}	−2	160	76	v s aq, alc; i eth
a264	**DL**-2-Amino-1-propanol	$CH_3CH(NH_2)CH_2OH$	75.11	4^1, 432	0.943	1.4495^{20}		173–176	83	v s aq, alc, eth
a265	*S*-(+)-2-Amino-1-propanol	$CH_3CH(NH_2)CH_2OH$	75.11	4^3, 735	0.965	1.4498^{20}		176	62	v s aq, alc, eth
a266	3-Amino-1-propanol	$H_2NCH_2CH_2CH_2OH$	75.11	4, 288	0.982	1.4610^{20}	10–12	188	79 (TOC)	s aq, alc
a267	2-Amino-1-propene-1,1,3-tricarbonitrile	$NCC(CN)=C(NH_2)CH_2CN$	132.13	Merck: 11, 495			171–173			s aq
a268	3-Aminopropyl-(diethoxy)methylsilane	$H_2N(CH_2)_3Si(CH_3)(OCH_2CH_3)_2$	191.4		0.916_4^{20}	1.427^{20}		88^{8mm}		
a269	1-(3-Aminopropyl)-imidazole		125.18	23^3, 577	1.049	1.5190^{20}			>110	
a270	*N*-(3-Aminopropyl)-iminodiethanol	$H_2N(CH_3)N(CH_2CH_2OH)_2$	162.23		0.1071	1.4980^{20}		170^{2mm}	137	
a271	*N*-(3-Aminopropyl)-morpholine		144.22		0.9872_{20}^{20}	1.4761^{20}	−15	224	98	misc aq, alc, bz
a272	*N*-(3-Aminopropyl)-2-pyrolidinone		142.20		1.014	1.500^{20}		123^{1mm}	>110	
a273	3-Aminopropyltriethoxysilane	$H_2N(CH_2)_3Si(OC_2H_5)_3$	221.37	0.9506_4^{20}	1.4225^{20}			217	104	
a274	3-Aminopropyltrimethoxysilane	$H_2N(CH_2)_3Si(OCH_3)_3$	179.29		1.01_4^{25}	1.420^{25}		80^{8mm}	83	
a275	2-Aminopyridine	$(C_5H_4N)NH_2$	94.12	22, 428			58.1	210.6	92	s aq, alc, bz, eth

a276	3-Aminopyridine	$(C_5H_4N)NH_2$	94.12	22, 431			64	250–252		s aq, alc, bz, eth
a277	4-Aminopyridine	$(C_5H_4N)NH_2$	94.12	22, 433			160–162	273		s aq, alc; sl s bz, eth
a278	2-Aminopyrimidine		95.11	24, 80			125–127	subl		v s aq
a279	4-Aminoquinaldine		158.20	22, 453			167–169	333		sl s aq; v s alc, eth, acet; s hot bz
a280	4-Aminosalicylic acid	$H_2NC_6H_3(OH)CO_2H$	153.14	14, 579			150–151			0.2 aq; 4.8 alc; s dil acids, alk; sl s eth
a281	5-Aminosalicylic acid	$H_2NC_6H_3(OH)CO_2H$	153.14	14, 579			280 d			
a282	2-Aminoterephthalic acid	$H_2NC_6H_3(CO_2H)_2$	181.15	14, 558			324 d			
a283	5-Amino-1,2,3,4-tetrazole hydrate		103.08	26, 403			204 d			

4-Aminophenyl phenyl ether, p70
Aminophenyl sulfones, d47, d48
3-Aminophthalhydrazide, a151
5-Amino-*m*-phthalic acid, a114
Aminopicolines, a222, a223

1-Aminopropane, p223
2-Aminopropane, i100
3-Amino-1-propene, a76
N-(3-Aminopropyl)diethanolamine, a270
6-Aminopurine, a66

2-Amino-3-pyridinol, a193
Aminopyrimidinediols, a152, a153
2-Aminosuccinamic acid, a301
Aminosuccinic acid, a304
6-Amino-2-thiouracil, a187



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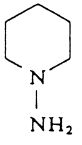

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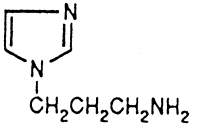

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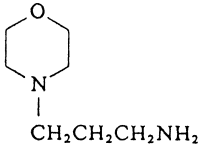

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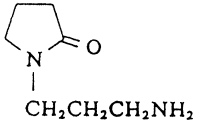

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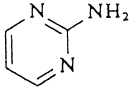

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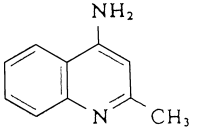

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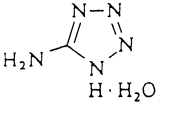

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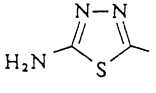
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
a284	2-Amino-1,3,4-thiadiazole		101.13	27, 624			190–192			
a285	2-Aminothiazole		100.14	27, 155			93			sl s aq, alc, eth; s hot aq, HCl
a286	2-Amino-2-thiazoline		100.14	27, 136			79–82			s HCl
a287	2-Aminothiophenol	$H_2NC_6H_4SH$	125.19	13, 397	1.170	1.6420^{20}	19–21	$72^{0.1mm}$	79	
a288	2-Aminotoluene-5-sulfonic acid	$H_2NC_6H_3(CH_3)SO_3H$	187.22	14, 726			>300			i aq[12]; v s hot aq
a289	3-Amino-1,2,4-triazole		84.08	26, 137			150–153			s aq, alc, chl
a290	5-Amino-1,3,3-trimethylcyclohexanemethylamine	$H_2N(C_6H_7)(CH_3)_3CH_2NH_2$	170.30		0.922	1.4880^{20}	10	247	>110	
a291	5-Amino-2,2,4-trimethylcyclopentanemethylamine		156.27		0.901	1.4733^{20}		221	97	
a292	11-Aminoundecanoic acid	$H_2N(CH_2)_{10}CO_2H$	201.31				190–192			
a293	Aniline	$C_6H_5NH_2$	93.12	12, 59	1.027^{20}_{20}	1.5863^{20}	−6	184–186	70	3.5 aq[25]; s acids; misc most org solv
a294	Aniline hydrochloride	$C_6H_5NH_2 \cdot HCl$	129.59	Merck: 12, 696	1.222		198	245	193 (CC)	100 aq; v s alc
a295	2-Anilinoethanol	$C_6H_5NHCH_2CH_2OH$	137.18	12, 182	1.085	1.5793^{20}		152^{10mm}	153	sl s aq; v s alc, chl, eth
a296	3-Anilinopropionitrile	$C_6H_5NHCH_2CH_2CN$	146.19				52–53		>110	
a297	Anthracene		178.23	5, 657	1.25^{27}_{4}		215-218	339–342	121 (CC)	1.5 alc; 1.6 bz; 1.2 chl; 3.1 CS_2; 0.5 eth; i aq
a298	9,10-Anthraquinone		208.20	7, 781	1.43^{20}_{4}		286	377	185 (CC)	0.44 alc[25]; 0.6 chl[20]; 0.2 bz[20]; 0.11 eth[25]
a299	Antipyrine		188.23	24, 27	1.088^{113}_{4}		111–114	319		100 aq; 77 alc; 100 chl; 2.3 eth
a300	L-(+)-Arabinose		150.13	31, 32			157–160			100 aq; 0.4 alc
a301	L-(+)-Arginine	$H_2NC(=NH)NH(CH_2)_3$-$CH(NH_2)CO_2H$	174.20	4, 420			d 240			15 aq[21]; sl s alc

a302	**L**-(+)-Ascorbic acid		176.12	18[3], 3038	1.65[25]		190–192			33 aq; 3.3 alc; 1 glyc; i bz, chl, eth, PE
a303	**L**-(+)-Asparagine	$H_2NCOCH_2CH(NH_2)CO_2H$	132.12	4, 476			235			3.5 aq[28]; s alkalis, acids; i alc, bz, eth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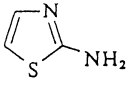
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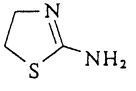
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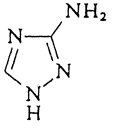
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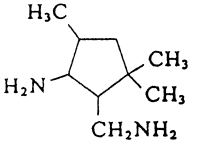
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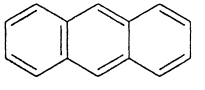
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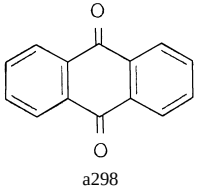
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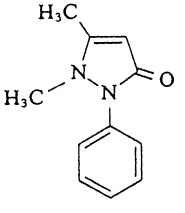
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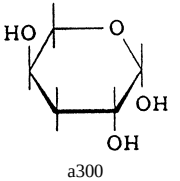
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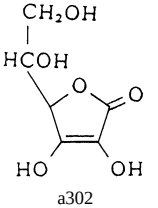
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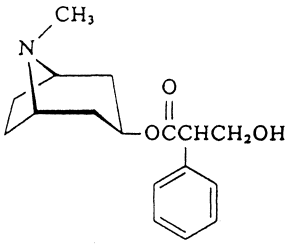
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
a304	L-(+)-Aspartic acid	$HO_2CCH_2CH(NH_2)CO_2H$	133.10	4, 472	$1.661^{12.5}$		270–272			0.45 aq; s alkalis, acids; i alc, eth
a305	Atropine		289.38	21, 27			114–116	subl 110 high vac		0.22 aq; 50 alc; 4 eth; 100 chl; 3.9 glyc; s bz, dil acids
a306	Aurintricarboxylic acid, triammonium salt		473.44	10^2, 775			225 d			v s aq
a307	2-Azacyclooctanone		127.19	21, 242			35–38	148^{10mm}	>110	
a308	2-Azacyclotridecanone		197.32				150–153			
a309	Azidotrimethylsilane	$(CH_3)_3SiN_3$	115.21		0.868	1.4140^{20}	−95	95–96	23	
a310	Azidotriphenylsilane	$(C_6H_5)_3SiN_3$	301.4				83–84	$100^{0.01mm}$		
a311	1-Aziridineethanol	$(C_2H_4N)CH_2CH_2OH$	87.12		1.088	1.4560^{20}		168	67	
a312	Azobenzene	$C_6H_5N{=}NC_6H_5$	182.23	16, 8	1.203_4^{20}		67–68	293		4.2 alc^{20}; s eth, HOAc
a313	2,2′-Azobis(2-methylpropionitrile)	$(CH_3)_2C(CN)N{=}NC(CN)(CH_3)_2$	164.21	4, 563				107 d		2 EtOH;[20] 5 MeOH;[20] can explode in acetone
a314	Azodicarbonamide	$H_2NCON{=}NCONH_2$	116.08	3, 123			225 d			i aq, alc; s hot aq
a315	4,4′-Azoxydianisole	$H_3OC_6H_4N{=}N(\rightarrow O)C_6H_4OCH_3$	258.28	16, 637			120			
a316	Azulene		128.17	5^2, 432			99–100	242		i aq; s org solvents
b1	Barbituric acid		128.09	24, 467			252 d			s hot aq, dil acids
b2	Basic fuchsin		337.86	13, 765	1.22		250 d			0.3 aq; s alc, acids
b3	Benzaldehyde	C_6H_5CHO	106.12	7, 174	1.050_4^{15}	1.5456^{20}	−26	179	63	0.3 aq; misc alc, eth
b4	Benzamide	$C_6H_5CONH_2$	121.13	9, 195	1.341^4		129–130	288–290		1.3 aq; 17 alc; 30 pyr
b5	Benzanilide	$C_6H_5CONHC_6H_5$	197.24	12, 262	1.315		163	117^{10mm}		i aq; 1.7 alc; sl s eth
b6	1,2-Benzanthracene		228.29	5, 718			155–157	437.6		sl s hot aq; s org solv
b7	2,3-Benzanthracene		228.29	5^2, 628	1.35		357 (Cu block)	subl		sl s most org solv
b8	Benzene	C_6H_6	78.11	5, 179	0.8787_4^{15}	1.5011^{20}	5.5	80.0	−11 (CC)	0.17 aq; misc most org solv
b9	Benzene-*1,3,5-d*$_3$	$C_6H_3D_3$	81.14	5^3, 518	0.908	1.4990^{20}		80	−11 (CC)	similar to ordinary benzene

b10	Benzene-$^{13}C_6$	$^{13}C_6H_6$	84.07		0.949	1.5010^{20}	5.5	80	−11 (CC)	similar to ordinary benzene
b11	Benzene-d_6	C_6D_6	84.16	5^3, 519	0.950	1.4986^{20}	6.8	79.1	−11 (CC)	similar to ordinary benzene
b12	Benzenearsonic acid	$C_6H_5AsO(OH)_2$	202.03	16, 868	1.760^{25}		162			2.5 aq; 2 alc; i chl

Aspirin, a56
Azabenzene, p257
Azacyclopentane, p280
Azacyclopropane, e146
1-Azanaphthalene, q3
Azelaic acid, n93
Azine, p257
Aziridine, e148
Azobis(isobutyronitrile), a313
Azole, p279
4,4′-Azoxyanisole, a315
Barbitol, d339
Behenyl alcohol, d817
Benzal bromide, d132
Benzal chloride, d273
Benzalphthalide, b105
Benzeneacetaldehyde, p77



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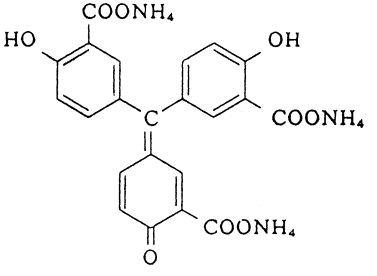

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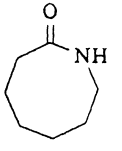

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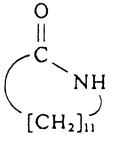

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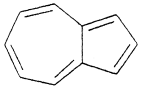
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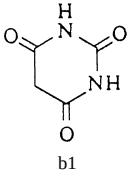

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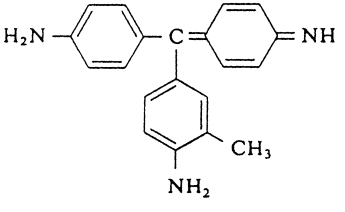

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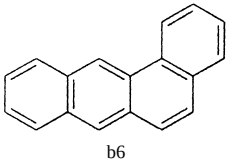
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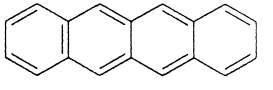
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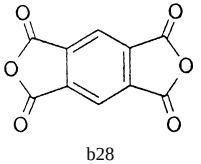
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b13	Benzeneboronic acid	$C_6H_5B(OH)_2$	121.94	16, 920			216			2.5 aq; 1.8 bz; 30 eth; 178 MeOH
b14	1,4-Benzenedicarbaldehyde	$C_6H_4(CHO)_2$	134.13	7, 675			113	248		i aq; 6 bz; 17 acet; 2 eth; 14 diox; 46 MeOH
b15	1,2-Benzenedicarbonyl dichloride	$C_6H_4(COCl)_2$	203.02	9, 834	1.409^{20}		15–16	280–282		d aq, alc; s eth
b16	1,4-Benzenedicarbonyl dichloride	$C_6H_4(COCl)_2$	203.02	9, 844			81	266	180	37 bz; 9 CCl_4
b17	1,3-Benzenedicarboxylic acid	$C_6H_4(COOH)_2$	166.13	9, 832			345–348	subl		0.012 aq; v s alc, HOAc; i bz, PE
b18	1,4-Benzenedicarboxylic acid	$C_6H_4(COOH)_2$	166.13	9, 841			subl 402			sl s alc; s alkalis; v sl s aq, chl, eth
b19	1,4-Benzenedimethanol	$C_6H_4(CH_2OH)_2$	138.17	6, 919	1.100^{117}		117–119	143^{1mm}	188	
b20	Benzenehexacarboxylic acid	$C_6(COOH)_6$	342.17	9, 1008			286 d			v s aq, alc
b21	Benzenesulfinic acid	$C_6H_5S(=O)OH$	142.16	11, 2			85	100 d		sl s aq; s alc, bz, eth
b22	Benzenesulfonamide	$C_6H_5SO_2NH_2$	157.19	11, 39			150–152			i aq; sl s alc; s eth
b23	Benzenesulfonic acid	$C_6H_5SO_2OH$	158.18	11, 26			50–51			v s aq, alc; sl s bz; i CS_2, eth
b24	Benzenesulfonyl chloride	$C_6H_5SO_2Cl$	176.62	11, 34	1.3842_{15}^{15}	1.5518^{20}	14.5	120^{10mm}	>110	i aq; s alc, eth
b25	Benzenesulfonyl fluoride	$C_6H_5SO_2F$	160.17	11[2], 23	1.3286_4^{20}	1.4920^{20}	−5	207–208	87	s alc, eth
b26	Benzenesulfonyl hydrazide	$C_6H_5SO_2NHNH_2$	172.21	11, 52			d 104			flammable solid
b27	1,2,4,5-Benzenetetracarboxylic acid	$C_6H_2(COOH)_4$	254.15	9, 997			276			1.5 aq; v s alc
b28	1,2,4,5-Benzenetetracarboxyl dianhydride		218.12	19, 196			283–286	397–400		
b29	1,2,3-Benzenetricarboxylic acid dihyrate	$C_6H_3(COOH)_3 \cdot 2H_2O$	246.18	9, 976			192 d			sl s aq; v s eth

b30	1,2,4-Benzenetricarboxylic acid	$C_6H_3(COOH)_3$	210.14	9, 997			231 d			2.1 aq; 25.3 alc; 7.9 acet; v s eth
b31	1,3,5-Benzenetricarboxylic acid	$C_6H_3(COOH)_3$	210.14	9, 978			>330			sl s aq; v s alc; s eth
b32	1,2,4-Benzenetricarboxylic anhydride		192.13	18, 468			161–163	245^{14mm}		50 acet; 22 EtOAc; 15 DMF
b33	1,3,5-Benzenetricarboxylic trichloride	$C_6H_3(COCl)_3$	265.48				35–36	180^{16mm}	>110	
b34	1,2,4-Benzenetriol	$C_6H_3(OH)_3$	126.11	6, 1087			141			v s aq, alc, eth, EtOAc
b35	Benzil	$C_6H_5CO—COC_6H_5$	210.23	7, 747	1.23_4^{15}		95	346–348		i aq; s alc, bz, chl, EtOAc, eth
b36	Benzil dioxime	$C_6H_5C(=NOH)$-$C(=NOH)C_6H_5$	240.25	7^3, 3816			(α) 240 (β) 214			i aq, HOAc, eth; sl s alc; s NaOH
b37	Benzilic acid	$(C_6H_5)_2C(OH)COOH$	228.24	10, 342			150			sl s aq; v s alc, eth hot aq
b38	Benzil monohydrazone	$C_6H_5C(=NNH_2)COC_6H_5$	224.26	7^1, 394			150–152			
b39	Benzimidazole		118.13	23, 131			170.5	>360		sl s aq, eth; v s alc
b40	7,8-Benzo-1,3-diaza-spiro[4,5]decane-2,4-dione		216.23	Merck: 12, 9372			268			s alc, HOAc
b41	1,4-Benzodioxan		136.15		1.142	1.5490^{20}		103^{6mm}	87	

Benzeneazobenzene, a312
Benzenecarbonitrile, b51
Benzenecarbonyl chloride, b66
Benzenecarboxyaldehyde, b3
Benzenecarboxylic acid, b44
Benzene-1,2-dicarboxylic acid, p168
Benzene-1,2-dicarboxylic anhydride, p169
1,4-Benzenediol, h86
Benzenemethanol, b78
1,2,3-Benzenetriol, t317
Benzenethiol, t156
Benzhydrazide, b71
Benzhydrol, d760
Benzhydrylamine, d761
Benzhydryl bromide, b326
p-Benzidine, b140
2-Benzimidazolethiol, m17
1,3-Benzodiazole, b39
1,2,3-Benzodioxaborole, c22
1,3-Benzodioxole, m251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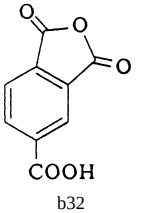
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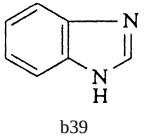
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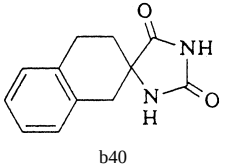
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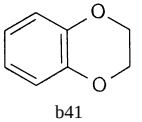
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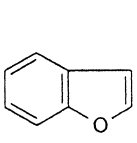
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b42	2,3-Benzofuran		118.13	17, 54	1.072	1.5660^{20}	<-18	173–175	56	i aq; misc alc, bz, eth, PE
b43	Benzofurazan-1-oxide		136.11	27^{1}, 740			69–71			
b44	Benzoic acid	C_6H_5COOH	122.12	9, 92	1.321		122.4	249	121 (CC)	0.29 aq[25]; 43 alc; 10 bz; 22 chl; 33 eth; 33 acet; 30 CS_2
b45	Benzoic anhydride	$(C_6H_5CO)_2O$	226.22	9, 164	1.1989_4^{15}		42	360	110	i aq; s alc, acet, chl bz, HOAc, EtOAc
b46	**DL**-Benzoin	$C_6H_5COCH(OH)C_6H_5$	212.25	8, 167	1.3100_4^{20}		137	194^{12mm}		s hot alc, acet; 20 pyr; sl s eth
b47	Benzoin ethyl ether	$C_6H_5CH(C_2H_5)COC_6H_5$	240.30	8, 174	1.1016_4^{17}	1.5727^{17}	62	195^{20mm}		s alc, bz, eth
b48	Benzoin isobutyl ether	$C_6H_5CH[OCH_2CH(CH_3)_2]$-$COC_6H_5$	268.36		0.985	1.5485^{20}		$133^{0.5mm}$	85	
b49	Benzoin methyl ether	$C_6H_5CH(OCH_3)COC_6H_5$	226.28	8, 174	1.1278_4^{14}		48	189^{15mm}	>110	v s alc, bz, eth
b50	α-Benzoinoxime	$C_6H_5CH(OH)C(=NOH)$-C_6H_5	227.26	8, 175			152–156			sl s aq; s alc, NH_4OH
b51	Benzonitrile	C_6H_5CN	103.12	9, 275	1.010	1.5289^{20}	-12.7	191	71	0.2 aq; misc org solv
b52	1,2-Benzophenanthrene		202.26	5, 718	1.274_4^{20}		258	448		i aq; s alc, eth
b53	Benzophenone	$C_6H_5COC_6H_5$	182.22	7, 411	1.1108_4^{18}	1.5975^{45}	48	305	>110	13.3 alc; 17 eth; s chl
b54	Benzophenone hydrazone	$C_6H_5C(=NNH_2)C_6H_5$	196.25	7, 417			95–98	230^{55mm}		
b55	1-Benzopyran-4(4*H*)-one		146.15	17, 327			55–60			
b56	1,2-Benzo[*a*]pyrene		252.32	Merck: 12, 1134			179	312^{10mm}		s bz; sl s alc
b57	4,5-Benzo[*e*]pyrene		252.32	Merck: 12, 1105			179			s bz
b58	1,4-Benzoquinone	$C_6H_4(=O)_2$	108.10	7, 609	1.318_4^{20}		116			sl s aq; s alc, hot bz, eth, hot PE; alkalis with dec
b59	Benzothiazole		135.19	Merck: 12, 1139	1.2460_4^{20}	1.6379^{20}	2	131^{34mm}	>110	sl s aq; v s alc, CS_2
b60	Benzo[*b*]thiophene		134.20	17, 59	1.1937^{40}	1.6302^{40}	32	221	>110	s alc, bz, chl, eth

b61	1,2,3-Benzotriazole		119.13	26, 38	1.238	1.6420^{20}	98.5	204 may explode		sl s aq; s alc, bz, chl, DMF
b62	Benzoxazole		119.12	27, 42		1.5594	30	182	58	sl s aq
b63	1-Benzoylacetone	$C_6H_5COCH_2COCH_3$	162.19	7, 680	1.090^{60}_{60}		60	260 sl d		sl s aq; v s alc, eth
b64	2-Benzoylbenzoic acid	$C_6H_5COC_6H_4COOH$	226.23	10, 747			129	265		sl s aq; v s alc, eth
b65	Benzoyl bromide	C_6H_5COBr	185.03	9, 195	1.5467^{20}	1.5883^{20}	−24	219	90	d aq, alc; misc eth
b66	Benzoyl chloride	C_6H_5COCl	140.57	9, 182	1.211^{20}_{4}	1.5537^{20}	−1.0	197.2	88 (CC)	d aq, alc; misc bz, eth CS_2
b67	Benzoyl cyanide	C_6H_5COCN	131.13	10, 659	1.106		32	206		i aq
b68	Benzoyl fluoride	C_6H_5COF	124.11	9, 181	1.140	1.4960^{20}	−28	161	48	d hot aq; v s alc, eth
b69	Benzoylformic acid	$C_6H_5COCOOH$	150.13	10, 654			67–69			

Benzofuroxan, b43
Benzoglyoxaline, b39
Benzoic acid hydrazide, b71
Benzhydroxylamine, a159
o-Benzoic sulfimide, s1
Benzo[*def*]phenanthrene, p255
Benzopyridine, q3
Benzoresorcinol, d443
2-Benzothiazolethiol, m19
Benzotrichloride, t251
Benzotrifluoride, t311
Benzoylamide, b4
Benzoylbenzene, b53
Benzoyl peroxide, d69
1,2-Benzophenanthrene, b6



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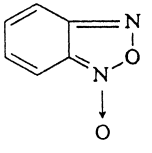

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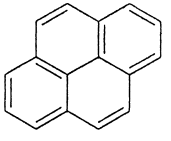
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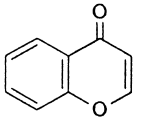

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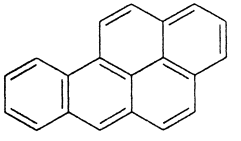
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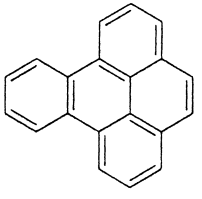
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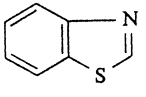

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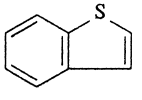

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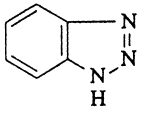

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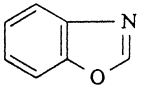


b62

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b70	*N*-Benzoylglycine	$C_6H_5CONHCH_2COOH$	179.18	9, 225			179			0.4 aq; 0.1 chl; 0.25 eth; sl s alc; i bz, PE
b71	Benzoylhydrazine	$C_6H_5CONHNH_2$	136.15	9, 319			117			
b71a	Benzoyl peroxide	$(C_6H_5CO)_2O_2$	242.23	9, 179			103–106	explodes		2.5 CS_2; s bz, chl, eth
b72	3-Benzoylpropanoic acid	$C_6H_5COCH_2CH_2COOH$	178.19	10, 696			117–119			sl s aq; s alc
b73	2-Benzoylpyridine	$C_6H_5CO(C_5H_4N)$	183.21	21, 330			44	317	150	
b74	3-Benzoylpyridine	$C_6H_5CO(C_5H_4N)$	183.21	21, 331			40	397	150	s alc, bz, eth
b75	4-Benzoylpyridine	$C_6H_5CO(C_5H_4N)$	183.21	21, 331			71	315	150	s alc, bz, eth
b76	Benzyl acetate	$CH_3CO_2CH_2C_6H_5$	150.18	6, 435	1.050_4^{25}	1.4998^{25}	−51.5	213.5	102 (CC)	i aq; misc alc, eth
b77	Benzyl acetoacetate	$CH_3COCH_2CO_2CH_2C_6H_5$	192.21	6, 438	1.112	1.5121^{20}		159^{10mm}	>110	
b77a	Benzylacetone	$C_6H_5CH_2CH_2COCH_3$	148.21	7, 314	0.989	1.5122^{20}		235	98	
b78	Benzyl alcohol	$C_6H_5CH_2OH$	108.14	6, 428	1.0453_4^{20}	1.5403^{20}	−15.2	205	93 (CC)	0.08 aq; misc alc, chl, eth
b79	Benzylamine	$C_6H_5CH_2NH_2$	107.16	12, 1013	0.983_4^{19}	1.5401^{20}	10	185	60	misc aq, alc, eth
b80	*N*-Benzylaminoethanol	$C_6H_5CH_2NHCH_2CH_2OH$	151.21	12, 1040	1.065	1.5435^{20}		156^{12mm}	>110	
b81	3-(Benzylamino)-propanonitrile	$C_6H_5CH_2NHCH_2CH_2CN$	160.22		1.024	1.5308^{20}			>110	
b82	*N*-Benzylbenzamide	$C_6H_5CH_2NHCH_2C_6H_5$	211.26				106			
b83	Benzyl benzoate	$C_6H_5CO_2CH_2C_6H_5$	212.25	9, 121	1.118_4^{25}	1.5681^{21}	21	323	148	misc alc, chl, eth
b84	2-Benzylbenzoic acid	$C_6H_5CH_2C_6H_4COOH$	212.24	9^2, 471			110–113			sl s aq; s alc, bz, chl, eth
b85	Benzyl bromide	$C_6H_5CH_2Br$	171.04	5, 306	1.4380_0^{22}	1.5752^{20}	−3.9	199	86	slowly dec aq
b86	Benzyl 2-bromoacetate	$BrCH_2CO_2CH_2C_6H_5$	229.08	6^1, 220	1.446	1.5440^{20}		170^{22mm}	>110	
b87	Benzyl-*tert*-butanol	$C_6H_5CH_2CH_2C(CH_3)_2OH$	164.25	6, 548		1.5090^{20}	31–33	144^{85mm}	>110	
b88	Benzyl butyl 1,2-phthalate	$C_6H_5CH_2O_2C_6H_4CO_2C_4H_9$	312.37	9^2, 594	1.119_{25}^{25}	1.5400^{20}			199	
b89	Benzyl carbamate	$C_6H_5CH_2OCONH_2$	151.17	6, 437			87–89	220 d		v s alc; sl s eth
b90	Benzyl chloride	$C_6H_5CH_2Cl$	126.59	5, 292	1.100_{20}^{20}	1.5381^{20}	−43 to −49	179	67	misc alc, chl, eth

b91	Benzyl chloroformate	$C_6H_5CH_2OCOCl$	170.60	6, 437	1.195	1.5190^{20}		103^{20mm}	91	dec aq; s eth
b92	Benzyl chlorothiol-formate	$C_6H_5CH_2SCOCl$	186.5		1.237_4^{30}	1.5711^{30}		$80^{0.13mm}$	118	
b93	Benzyl cinnamate	$C_6H_5CH{=}CHCO_2CH_2C_6H_5$	238.29	9, 584			39	200^{5mm}	>110	s alc, eth; i aq, glyc
b94	*S*-Benzyl-**L**-cysteine	$C_6H_5CH_2SCH_2CH(NH_2)$-COOH	211.28	6, 465			214 d			
b95	Benzyl *N*,*N*-dimethyl-dithiocarbamate	$(CH_3)_2NCS_2CH_2C_6H_5$	211.35				41		>110	
b96	Benzyldimethylstearyl-ammonium chloride hydrate	$C_6H_5CH_2N[(CH_2)_{17}CH_3]$-$(CH_3)_2Cl \cdot H_2O$	442.18	12^3, 2212			67–69			
b96a	*N*-Butyl-*N*-ethylaniline	$C_6H_5N(CH_2C_6H_5)C_2H_5$	211.31	12, 1026	1.029	1.5950^{20}		164^{6mm}	>110	
b97	Benzyl ethyl ether	$C_6H_5CH_2OC_2H_5$	136.20	Merck: 12, 1168	0.9478^{20}	1.4955^{20}		186		misc alc, eth; i aq
b98	*N*-Benzylformamide	$C_6H_5CH_2NHCHO$	135.17	12, 1043			61			
b99	Benzyl formate	$C_6H_5CH_2O_2CH$	136.15	Merck: 12, 1169	1.081_4^{20}			203		i aq; s alc
b100	Benzyl 4-hydroxy-benzoate	$HOC_6H_4CO_2CH_2C_6H_5$	228.25	10,*3*, 311			110–112			
b101	*O*-Benzylhydroxyl-amine hydrochloride	$C_6H_5CH_2ONH_2 \cdot HCl$	159.62	6, 440				238 subl	>110	
b102	Benzylidineaniline	$C_6H_5N{=}CHC_6H_5$	181.24	12, 195	1.045_4^{50}		56	300	>110	s alc, chl, CS_2
b103	Benzylidenemalono-nitrile	$C_6H_5CH{=}C(CN)_2$	154.17	9, 895			83–85			
b104	*N*-Benzylidenemethyl-amine	$C_6H_5CH{=}NCH_3$	119.17	7, 213	0.967	1.5520^{20}		80^{18mm}	>112	

Benzylaniline, p93
Benzylbenzene, d759
Benzyl cyanide, p82
Benzyl disulfide, d72
Benzyl ethanoate, b76
N-Benzylethanolamine, b80
Benzyl ether, d73
Benzylideneacetone, p94
Benzylideneacetophenone, c23
Benzylidene chloride, d273

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

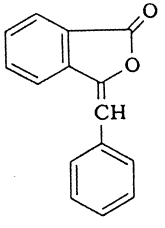
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b105	3-Benzylidene-phthalide		124.21	17, 376			99–102			
b106	Benzyl mercaptan	$C_6H_5CH_2SH$	222.24	6, 453	1.058^{20}	1.5751^{20}		206^{30mm}	>110	
b107	Benzyl methacrylate	$H_2C{=}C(CH_3)CO_2CH_2C_6H_5$	176.22	6^3, 1481	1.040	1.5120^{20}		98^{4mm}	77	
b108	*N*-Benzylmethylamine	$C_6H_5CH_2NHCH_3$	138.23	12, 1019	0.939	1.5230^{20}		184–189	77	
b109	3-(*N*-Benzyl-*N*-methyl-amino)-1,2-propane-diol	$C_6H_5CH_2N(CH_3)CH_2$-CH(OH)CH_2OH	195.26		1.084	1.5341^{20}		206^{30mm}	>110	
b110	Benzyl methyl sulfide	$C_6H_5CH_2SCH_3$	138.23	6, 453	1.015	1.5620^{20}		195–198	73	
b111	1-Benzyl-3-methyl-2-thiourea	$C_6H_5CH_2NHC(=S)NHCH_3$	180.27	12, 1052			74–76			
b112	Benzyl nicotinate	$(C_5H_4N)CO_2CH_2C_6H_5$	213.24	22,*3*, 366	1.165	1.5700^{20}	21–23	189^{12mm}	>110	
b113	4-Benzyloxybenz-aldehyde	$C_6H_5CH_2OC_6H_4CHO$	212.25	8, 73			73–74			
b114	4-Benzyloxybenzyl alcohol	$C_6H_5CH_2OC_6H_4CH_2OH$	214.26				86–87			
b115	2-Benzyloxyethanol	$C_6H_5CH_2OCH_2CH_2OH$	152.20	6^2, 413	1.07_{20}^{20}	1.5210^{20}		265	129	0.4 aq
b116	4-Benzyloxy-3-meth-oxybenzaldehyde	$C_6H_5CH_2OC_6H_4(OCH_3)CHO$	242.29				63–65			
b117	4-(Benzyloxymethyl)-2,2-dimethyl-1,3-dioxolane		222.28	19^2, 73	1.051	1.4940^{20}		$91^{0.1mm}$	>110	
b118	Benzyl phenyl sulfide	$C_6H_5CH_2SC_6H_5$	200.30	6, 454			41–44	197^{27mm}	>110	i aq; sl s alc; s eth
b119	1-Benzylpiperazine		176.26		1.014	1.5467^{20}			>110	s aq, alc, eth
b120	4-Benzylpiperidine		175.28	20, 296	0.997	1.5379^{20}	6–7	279	>110	
b121	1-Benzyl-4-piperidone		189.26		1.021	1.5399^{20}		134^{7mm}	>110	
b122	2-Benzylpyridine	$C_6H_5CH_2(C_5H_4N)$	169.23	20, 425	1.054	1.5790^{20}	8–10	276	125	i aq; v s alc, eth
b123	4-Benzylpyridine	$C_6H_5CH_2(C_5H_4N)$	169.23	20, 426	1.061_0^{20}	1.5818^{20}		287	115	s alc; v s eth
b124	1-Benzyl-2-pyrrolidi-none		175.23		1.095	1.5525^{20}			>110	
b125	Benzyl salicylate	$HOC_6H_4CO_2CH_2C_6H_5$	228.25	Merck: 12, 1181	1.175^{20}			208^{25mm}		sl s aq; misc alc, eth
b126	Benzyl thiocyanate	$C_6H_5CH_2SCN$	149.22	6, 460			43	235	>110	i aq; s alc; v s eth
b127	Benzyltributyl-ammonium chloride	$C_6H_5CH_2N(C_4H_9)_3^+Cl^-$	312.94				164 d			

b128	Benzyltrichlorosilane	$C_6H_5CH_2SiCl_3$	225.28	16, 912	1.288_4^{20}	1.5250^{20}		142^{100mm}	93	
b129	Benzyltriethoxysilane	$C_6H_5CH_2Si(OC_2H_5)_3$	254.40		0.986_4^{20}			175^{70mm}		
b130	Benzyltriethylammonium chloride	$C_6H_5CH_2N(C_2H_5)_3^+Cl^-$	227.78	12, 1021			185 d			
b131	Benzyltrimethylammonium chloride	$C_6H_5CH_2N(CH_3)_3^+Cl^-$	185.70	12, 1021			239 d		none	
b132	Benzyltrimethylsilane	$C_6H_5CH_2Si(CH_3)_3$	164.32	16,*1*, 526	0.8933^{20}	1.4941^{20}		190	57	
b133	Betaine	$(CH_3)_3N^+CH_2COO^-$	117.15	4, 347			dec 310			160 aq; 55 MeOH; 8.7 EtOH

Benzyl methyl ketone, p147
Benzyloxyamine, b101

Benzylphenol, h116
o,o-Bibenzoic acid, b141

Bibenzyl, d752
Bicine, b199



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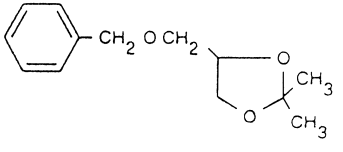

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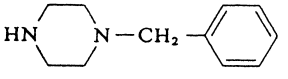

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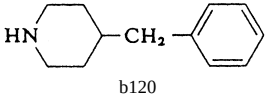

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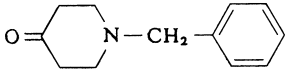

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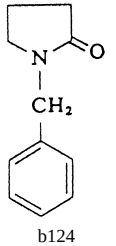


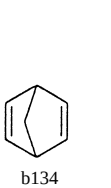
b124

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

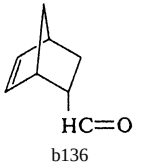
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b134	Bicyclo[2.2.1]hepta-2,5-diene		92.14		0.909^{20}	1.4707^{20}	−20	89	−11	i aq; s PE
b135	Bicyclo[2.2.1]-2-heptene		94.16				44–46	96	−15	s eth
b136	Bicyclo[2.2.1]-2-heptene-2-carbaldehyde		122.16		1.108	1.4883^{20}		70^{12mm}	51	
b137	Biguanide	$H_2NC(=NH)NHC(=NH)NH_2$	101.11	3, 93			130	dec 142		s aq, alc; i bz, chl, eth
b138	Biphenyl	$C_6H_5—C_6H_5$	154.20	5, 578	0.991_4^{75}	1.588^{77}	69–71	256	113 (CC)	i aq; s alc, eth
b139	4-Biphenylcarboxylic acid	$C_6H_5—C_6H_4COOH$	198.22	9, 671			226	subl		v s alc, eth; s bz; i aq
b140	4,4′-Biphenyldiamine	$H_2NC_6H_4—C_6H_4NH_2$	184.24	13, 214			120	*ca.* 400		s alc; 2 eth; 20 hot alc
b141	2,2′-Biphenyldicarboxylic acid	$HOOCC_6H_4—C_6H_4COOH$	242.23	9, 922			228–229			0.06 aq; s org solvents
b142	4-Biphenylsulfonic acid	$C_6H_5—C_6H_4SO_3H$	234.26				138			
b143	2-Biphenylyl glycidyl ether		226.28				30–32	$120^{0.1mm}$		
b144	2,2-Bis[4-(allyloxy)-phenyl]-propane	$H_2C=CHCH_2OC_6H_4C(CH_3)_2C_6H_4—OCH_2CH=CH_2$	308.42		1.022	1.5636^{20}			>110	
b145	*N,N′*-Bis(3-aminopropyl)ethylenediamine	$H_2N(CH_2)_3NHCH_2CH_2NH(CH_2)_3NH_2$	174.29		0.952	1.4910^{20}		160^{5mm}	>110	
b146	*N,N′*-Bis(3-aminopropyl)piperazine		200.33	23^2, 12	0.973	1.5015^{20}	15	152^{2mm}	162	
b147	*N,N′*-Bis(3-aminopropyl)-1,3-propanediamine	$H_2N(CH_2)_3NHCH_2CH_2CH_2NH(CH_2)_3NH_2$	188.32	4^4, 1278	0.920	1.4915^{20}		103^{1mm}		
b148	Bis(2-bromoethyl) ether	$BrCH_2CH_2OCH_2CH_2Br$	231.92					107^{20mm}		
b149	1,3-Bis(bromoethyl)-tetramethyldisiloxane	$[BrCH_2Si(CH_3)_2]_2O$	320.17		1.3918_4^{20}	1.4719^{20}		104^{15mm}		

b150	2,2-Bis(bromomethyl)-1,3-propanediol	$HOCH_2CH(CH_2Br)_2CH_2OH$	261.95	1^{1}, 251			114			
b151	Bis(2-butoxyethyl)-ether	$(C_4H_9OCH_2CH_2)_2O$	218.34		0.8853_{20}^{20}	1.4240^{20}	−60.2	256	118	0.3 aq; misc alc, esters, eth, CCl_4 ketones
b152	Bis[2-(2-butoxyethoxy)-ethyl] adipate	$[-CH_2CH_2CO_2(CH_2CH_2O)_2-(CH_2)_3CH_3]_2$	434.58	2^{3}, 1718	1.010	1.4480^{20}	−11		110	
b153	2,5-Bis(5-*tert*-butyl-2-2′-benzoxazolyl)-thiophene		430.57				201			
b154	Bis(*sec*-butyl) disulfide	$[CH_3CH_2CH(CH_3)]_2S_2$	178.36	1^{3}, 1549	0.957	1.4920^{20}		164^{739mm}	112	
b155	Bis(*tert*-butyl) disulfide	$(CH_3)_3CSSC(CH_3)_3$	178.36	1, 379	0.909	1.4930^{20}		204	79	
b156	1,1-Bis(*tert*-butylperoxy)cyclohexane	$C_6H_{10}[OOC(CH_3)_3]_2$	260.38		0.970	1.4570^{20}		54^{15mm}	90	

Bicyclo[4.4.0]decane, d2, d3
Bicyclo[5.3.0]decapentane, a316
Biformyl, g28
Biphenol, d436
Biphenylamines, a130, a131
2,2′-Bipyridine, d790
Bis(2-aminoethyl)amine, d362
Bis(4-aminophenyl)ether, o67
1,3-Bis(aminomethyl)cyclohexane, c349
1,2-Bis(benzylamino)ethane, d74
Bis(3-*tert*-butyl-4-hydroxy-5-ethylphenyl) sulfide, t140


b134


b135



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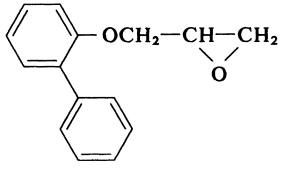

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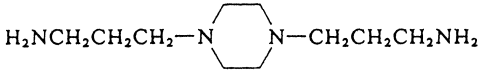

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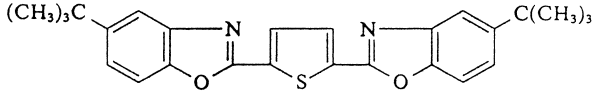


b153

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b157	2,5-Bis(*tert*-butylperoxy)-2,5-dimethylhexane	$[(CH_3)_3COOC(CH_3)_2CH_2\text{-}]_2$	290.45		0.877	1.4230^{20}		57^{7mm}	41	
b158	2,5-Bis(*tert*-butylperoxy)-2,5-dimethyl-3-hexyne	$(CH_3)_3COOC(CH_3)_2C{\equiv}C\text{-}C(CH_3)_2OOC(CH_3)_3$	286.41	1[4], 2701	0.881	1.4320^{20}		67^{2mm}	85	
b159	Bis[1-(*tert*-butylperoxy)-1-methylethyl-benzene	$C_6H_4[C(CH_3)_2OOC(CH_3)_3]_2$	338.49				44–48			flammable solid oxidizer
b160	1,1-Bis(*tert*-butylperoxy)-3,3,5-trimethyl-cyclohexane	$[(CH_3)_3COO]_2C_6H_7(CH_3)_3$	302.46		0.906	1.4410^{20}			87	
b161	1,2-Bis(2-chloroethoxy)ethane	$(ClCH_2CH_2OCH_2\text{-})_2$	187.07	1[3], 2079	1.197_4^{20}	1.4610^{20}		235	121	
b162	Bis(2-chloroethoxy)-methylsilane	$H(CH_3)Si(OCH_2CH_2Cl)_2$	203.1		1.1643_4^{20}	1.4431^{20}		97^{18mm}		
b163	Bis(2-chloroethyl) ether	$ClCH_2CH_2OCH_2CH_2Cl$	143.01	1[2], 335	1.2220_{20}^{20}	1.4575^{20}	−50 to −52	178.5	55	s most org solvents
b164	Bis(2-chloroethyl)-*N*-methylamine	$CH_3N(CH_2CH_2Cl)_2$	156.07		1.118_4^{25}		−60	75^{10mm}		v sl s aq; misc most org solvents
b165	Bis(chloromethyl)dimethylsilane	$(CH_3)_2Si(CH_2Cl)_2$	157.12	4[3], 1845	1.975_4^{20}	1.4600^{20}		160	46	
b165a	Bis(chloromethyl) ether	$ClCH_2OCH_2Cl$	114.96	Merck: 12, 3119	1.315_4^{20}	1.4346	−41.5	106		dec aq
b166	Bis(2-chloro-1-methyl)ethyl ether	$ClCH_2CH(CH_3)OCH(CH_3)\text{-}CH_2Cl$	171.07		1.1122_{20}^{20}			187.3	85	
b167	1,3-Bis(chloromethyl)-tetramethyldisiloxane	$[ClCH_2Si(CH_3)_2]_2O$	231.3	4[3], 1864	1.050	1.4405^{20}		205	73	
b168	Bis(4-chlorophenoxy)-acetic acid	$(ClC_6H_4O)_2CHCOOH$	313.14				140–142			

b169	2,2-Bis(4-chlorophenyl)-1,1-dichloroethane	$(ClC_6H_4)_2CHCHCl_2$	320.05	5^{3}, 1830			110			similar to b168
b170	1,1-Bis(4′-chlorophenyl)ethanol	$(ClC_6H_4)_2C(OH)CH_3$	267.16	6^{3}, 3396			69			s org solvents
b171	Bis(4-chlorophenyl) sulfone	$ClC_6H_4SO_2C_6H_4Cl$	287.16	6, 327			145–148	250^{10mm}		
b172	Bis(4-chlorophenyl) sulfoxide	$ClC_6H_4S(O)C_6H_4Cl$	271.17	6^{1}, 149			141–144			
b173	1,1-Bis(4-chlorophenyl)-2,2,2-trichloroethane	$(ClC_6H_4)_2CHCCl_3$	354.49	5^{3}, 1833			109–111			58 acet; 78 bz; 45 chl; v s pyr, 1,4-dioxane
b174	1,2-Bis(dichloromethylsilyl)ethane	$[\text{-}CH_2Si(CH_3)Cl_2]_2$	256.11	4^{4}, 192	1.263	1.4760^{20}	33–35	210	90	
b175	1,3-Bis(dichloromethyl)tetramethyldisiloxane	$[ClCH(CH_3)_2Si]_2O$	300.16		1.2213_4^{20}	1.4660^{20}		149^{40mm}		
b176	*N*,*N*-Bis(2,2-diethoxyethyl)methylamine	$[(C_2H_5O)_2CHCH_2]_2NCH_3$	263.38	4, 311	0.945	1.4259^{20}		222^{244mm}	60	
b177	4,4′-Bis(diethylamino)benzophenone	$[(C_2H_5)_2NC_6H_4]_2C{=}O$	324.47	14, 98			95			
b178	4,4′-Bis(dimethylamino)benzophenone	$(CH_3)_2NC_6H_4]_2C{=}O$	268.35	14, 89			172	>360 d		s alc, warm bz; v sl s eth; i aq
b179	Bis(dimethylamino)dimethylsilane	$[(CH_3)_2N]Si(CH_3)_2$	146.31	4^{4}, 4143	0.810^{22}	1.4170^{20}	−98	128–129	−7	
b180	1,3-Bis(dimethylamino)-2-propanol	$[(CH_3)_2NCH_2]_2CHOH$	146.23	4, 290	0.897	1.4422^{20}			>110	
b181	2,4-Bis(α,α-dimethylbenzyl)phenol	$[C_6H_5C(CH_3)_2]_2C_6H_3OH$	330.47	6^{4}, 5076			63–65	206^{15mm}		
b182	1,1-Bis(3,4-dimethylphenyl)ethane	$[(CH_3)_2C_6H_3]_2CHCH_3$	238.38	5^{3}, 1908	0.982	1.5640^{20}		174^{5mm}	>110	
b183	Bis(dimethylthiocarbamyl) disulfide	$[(CH_3)_2NC(=S)S\text{-}]_2$	240.43	4, 76	1.29		155–156			s alc, eth; sl s bz, acet; i aq

Bis(4-chlorophenyl) sulfone, c223

Bis(2-cyanoethyl) ether, a62

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

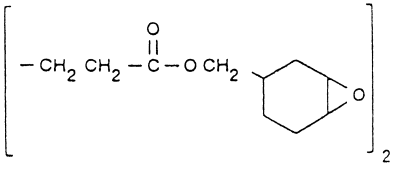
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b184	Bis(3,4-epoxycyclohexylmethyl) adipate		366.46		1.149	1.4930			>110	
b185	1,4-Bis(2,3-epoxypropoxy)butane	$[H_2C\!-\!CHCH_2OCH_2CH_2-]_2$ (O)	202.25		1.049	1.4530^{20}		160^{11mm}	>110	
b186	Bis(2-ethoxyethyl) ether	$(C_2H_5OCH_2CH_2)_2O$	162.23	1^2, 519	0.907_4^{20}	1.4110^{20}	−45	188	82	v s aq, alc, org solvents
b187	Bis(2-ethylhexyl) adipate	$[-CH_2CH_2CO_2CH(C_2H_5)-(CH_2)_3CH_3]_2$	370.58	2^3, 1715	0.990	1.4425^{20}		167^{1mm}	>110	
b188	Bis(2-ethylhexyl)-amine	$[CH_3(CH_2)_3CH(C_2H_5)-(CH_2)_3CH_3]_2$	241.46	4^3, 388	0.805	1.4425^{20}		123^{5mm}	>110	
b189	Bis(2-ethylhexyl) chlorendate		613.28		1.240	1.500^{20}		$233^{0.3mm}$	>110	
b190	Bis(2-ethylhexyl) decanedioate	$CH_3(CH_2)_3CH(C_2H_5)CH_2-OOC(CH_2)_8COOCH_2-CH(C_2H_5)(CH_2)_3CH_3$	426.66		0.9119_{25}^{25}	1.4496^{25}				
b191	Bis(2-ethylhexyl) hydrogen phosphate	$[CH_3(CH_2)_3CH(C_2H_5)-CH_2O]_2P(O)OH$	322.43	1^4, 1786	0.965	1.4430^{20}	−60	209^{10mm}	>110	
b192	Bis(2-ethylhexyl) hydrogen phosphite	$[CH_3(CH_2)_3CH(C_2H_5)-CH_2O]_2POH$	306.43		0.916	1.4420^{20}			>110	
b193	Bis(2-ethylhexyl) *o*-phthalate	$[CH_3(CH_2)_3CH(C_2H_5)-CH_2OOC]_2C_6H_4$	390.56	Merck: 12, 1291	0.9843^{20}	1.4859^{20}	−50 to −55	384	218	0.01 aq
b194	Bis(2-ethylhexyl) 1,4-phthalate	$[CH_3(CH_2)_3CH(C_2H_5)-CH_2OOC]_2C_6H_4$	390.56	9,*4*, 3306	0.980	1.4900^{20}	30–34	400	>110	
b195	Bis(4-fluorophenyl)-methane	$(FC_6H_4)_2CH_2$	204.22	5^3, 1789	1.145	1.5362^{20}	29–30	260^{742mm}	>110	
b196	Bis(hexamethylene)-triamine	$[H_2N(CH_2)_6]_2NH$	215.39				33–36	165^{4mm}	>110	
b197	1,4-Bis(2-hydroxyethoxy)-2-butyne	$HOCH_2CH_2OCH_2C{\equiv}CCH_2-OCH_2CH_2OH$	174.20		1.144	1.4850^{20}			>110	
b198	Bis(2-hydroxyethyl) ether	$HOCH_2CH_2OCH_2CH_2OH$	106.12	1, 468	1.1184_{20}^{20}	1.4460^{20}	−10.4	246	118	misc aq, alc, acet, eth
b199	*N*,*N*-Bis(2-hydroxyethyl)glycine	$(HOCH_2CH_2)_2NCH_2COOH$	163.17	Merck: 12, 1248			193–195			17.9 aq[0]

b200	2,6-Bis(hydroxymethyl)-*p*-cresol	$CH_3C_6H_2(CH_2OH)_2OH$	168.19	6, 1127			128–130			
b201	2,2-Bis(hydroxymethyl)propanoic acid	$(HOCH_2)_2C(CH_3)COOH$	134.13	3, 401			181–185			s aq, MeOH; sl s acet; i bz
b202	4,8-Bis(hydroxymethyl)tricyclo-[5.2.1.$0^{2,6}$]decane		196.29	6^4, 5538		1.5280^{20}			110	
b203	4,4-Bis(4-hydroxyphenyl)pentanoic acid	$CH_3C(C_6H_4OH)_2CH_2CH_2COOH$	286.33	Merck: 12, 3370			171–172 higher melting form			s hot aq, acet, alc, HOAc, MeEtKe
b204	Bis(2-hydroxypropyl) ether	$HO(CH_2)_3O(CH_2)_3OH$	134.18	1^2, 537	1.0252^{20}_{20}	1.4410^{20}		231.8	137	misc aq, alc
b205	1,3-Bis(isocyanatomethyl)benzene	$C_6H_4(CH_2NCO)_2$	188.19	13^3, 334	1.202	1.5910^{20}	−7	130^{2mm}	>110	
b206	1,3-Bis(isocyanatomethyl)cyclohexane	$C_6H_{10}(CH_2NCO)_2$	194.24		1.101	1.4850^{20}			>110	
b207	1,3-Bis(1-isocyanato-1-methylethyl)-benzene	$C_6H_4[C(CH_3)_2NCO]_2$	244.30		1.060	1.5110^{20}		$106^{0.9mm}$	153	
b208	Bis(2-mercaptoethyl) ether	$(HSCH_2CH_2)_2O$	138.25		1.114		−80	217	98	
b209	Bis(2-mercaptoethyl) sulfide	$(HSCH_2CH_2)_2S$	154.32		1.183	1.5961^{20}		136^{10mm}	90	

Bis(2-ethylhexyl) sebacate, b190
1,2-Bis(2-hydroxyethoxy)ethane, t280

Bis(2-hydroxyethyl) sulfide, t144
2,2-Bis(hydroxymethyl)-1,3-propanediol, p19

Bis(4-hydroxyphenyl) sulfide, t145
4,4-Bis(hydroxyphenyl)valeric acid, b203



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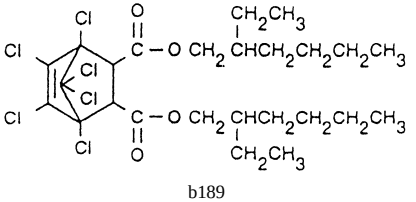

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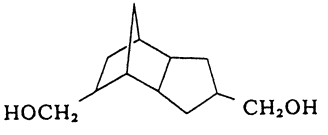


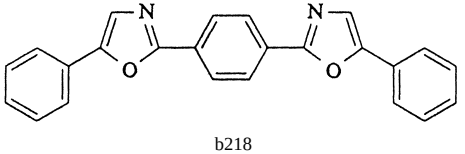
b202

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b210	1,4-Bis(methanesulfonoxy)butane	$(CH_3SO_2OCH_2CH_2-)_2$	246.30				115–117			sl hyd aq; 0.1 alc; 1.4 acet
b211	1,2-Bis(methoxyethoxy)ethane	$(CH_3OCH_2CH_2OCH_2-)_2$	178.23		0.990_4^{20}	1.4224^{20}	−45	216	110	misc aq
b212	Bis[2-(2-methoxyethoxy)ethyl] ether	$(CH_3OCH_2CH_2OCH_2CH_2)_2O$	228.28	1^3, 2107	1.0087_4^{20}	1.4330^{20}	−27	275	140	s aq
b213	Bis(2-methoxyethyl)amine	$(CH_3OCH_2CH_2)_2NH$	133.19	4^3, 691	0.902	1.4190^{20}		172	58	
b214	Bis(2-methoxyethyl) ether	$(CH_3OCH_2CH_2)_2O$	134.18	1^2, 520	0.9440^{25}	1.4043^{25}	−64 to −68	162	67	misc aq
b214a	2,2-Bis(4-methoxyphenyl)-1,1,1-trichloroethane	$(CH_3OC_6H_4)_2CHCCl_3$	345.66	6, 1007			86–88			v sl s aq; s alc
b215	Bis(2-methylallyl) carbonate	$[H_2C{=}C(CH_3)CH_2O]_2C{=}O$	170.21		0.943	1.4370^{20}		202	72	
b216	Bis(3-nitrophenyl) disulfide	$O_2NC_6H_4SSC_6H_4NO_2$	308.33	6, 339			83			i aq; s alc; v s eth
b217	Bis(octadecyl)pentaerythritol diphosphite	$[C_{18}H_{37}OP(OCH_2)_2-]_2$	721.01		0.925	1.457	40		261	
b218	1,4-Bis(5-phenyloxazol-2-yl)benzene		364.40				244			
b219	*N,N′*-Bis(salicylidene)-1,4-butanediamine	$HOC_6H_4CH{=}N(CH_2)_4$-$N{=}CHC_6H_4OH$	296.37	8^3, 163			88–90			
b220	*N,N′*-Bis(salicylidene)-ethylenediamine	$(-CH_2N{=}CHC_6H_4OH)_2$	268.32	8, 48			128			
b221	*N,N′*-Bis(salicylidene)-1,6-hexanediamine	$HOC_6H_4CH{=}N(CH_2)_6$-$N{=}CHC_6H_4OH$	324.44	8^3, 165			69			
b222	Bis(*p*-tolyl) disulfide	$CH_3C_6H_4SSC_6H_4CH_3$	246.39	6, 425			43–46			i aq; s alc; v s eth
b223	Bis(*p*-tolyl) sulfoxide	$CH_3C_6H_4S(\rightarrow O)C_6H_4CH_3$	230.33	6, 419			94–96			v s alc, bz, chl, eth
b224	Bis(tributyltin) oxide	$(C_4H_9)_3SnOSn(C_4H_9)_3$	596.08		1.170	1.4860^{20}		180^{2mm}	>110	
b225	1,4-Bis(trichloromethyl)benzene	$Cl_3CC_6H_4CCl_3$	312.84	5, 385			108–110			i aq; 26 acet; 38 bz

b226	Bis(2,4,5-trichlorophenyl) disulfide	$Cl_3C_6H_2SSC_6H_2Cl_3$	425.01				140–144		
b227	1,2-Bis(trichlorosilyl)ethane	$Cl_3SiCH_2CH_2SiCl_3$	296.94	4^4, 4266	1.483_4^{20}	1.4750^{20}	24.5	202	65
b228	3,5-Bis(trifluoromethyl)aniline	$(F_3C)_2C_6H_3NH_2$	229.13		1.467	1.4340^{20}		85^{15mm}	83
b229	1,3-Bis(trifluoromethyl)benzene	$(F_3C)_2C_6H_4$	214.11	5^3, 834	1.3790^{25}	1.3916^{25}		116	26
b230	*N*,*O*-Bis(trimethylsilyl)acetamide	$CH_3—C(=N—Si(CH_3)_3)(—O—Si(CH_3)_3)$	203.43		0.832_4^{20}	1.4170^{20}		73^{35mm}	11
b231	Bis(trimethylsilyl)acetylene	$(CH_3)_3SiC{\equiv}CSi(CH_3)_3$	170.41		0.770_4^{20}	1.4270^{20}		137	2
b232	Bis(trimethylsilyl)formamide	$HC(=NSi(CH_3)_3)(OSi(CH_3)_3)$	189.41		0.885	1.4381^{20}		55^{13mm}	
b233	*N*,*O*-Bis(trimethylsilyl)hydroxylamine	$(CH_3)_3SiONHSi(CH_3)_3$	177.40		0.830	1.4112^{20}		80^{100mm}	28
b234	1,2-Bis(trimethylsilyloxy)ethane	$(CH_3)_3SiOCH_2CH_2OSi(CH_3)_3$	206.43		0.842	1.4034^{20}		166	46
b235	*N*,*O*-Bis(trimethylsilyl)trifluoroacetamide	$F_3C[=NSi(CH_3)_3]OSi(CH_3)_3$	257.40		0.969	1.3839^{20}	−10	50^{14mm}	23
b236	1,3-Bis(trimethylsilyl)urea	$(CH_3)_3SiNHCONHSi(CH_3)_3$	204.42				232 dec		

1,2-Bis(2-methoxyethoxy)ethane, t282
Bis(phenylmethyl) disulfide, d72
Bis-tris propane, b237
2-Bornanone, c3



b218

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

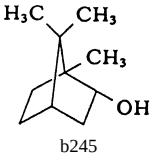
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b237	1,3-Bis[tris(hydroxymethyl)methylamino]propane	$CH_2[CH_2NHC(CH_2OH)_3]_2$	282.34	4^3, 859			170			s aq
b238	Biuret	$H_2NC(=O)NHC(=O)NH_2$	103.08	3, 70	1.467_4^{-5}		anhyd 110	dec 190		v s alc; 2 aq[25]
b239	Borane-*tert*-butylamine	$(CH_3)_3CNH_2 \cdot BH_3$	86.97				100 dec			
b240	Borane-*N*,*N*-diethylaniline	$C_6H_5N(C_2H_5)_2 \cdot BH_3$	163.07				−30		21	
b241	Borane-*N*,*N*-diisopropylethylamine	$[(CH_3)_2CH]_2C_2H_5 \cdot BH_3$	143.08		0.822	1.4600^{20}	15–17		40	
b242	Borane-dimethylamine	$(CH_3)_2NH \cdot BH_3$	58.92				36		43	
b243	Borane-dimethyl sulfide	$(CH_3)_2S \cdot BH_3$	75.97		0.801				18	
b244	Borane-pyridine	$C_5H_4N \cdot BH_3$	92.93		0.920	1.5320^{20}	10–11		21	
b245	(1*S*-*endo*)-(−)-Borneol		154.25	6, 72	1.011_4^{20}		204	210^{779mm}	65	i aq; 176 alc; s eth
b246	(−)-1-Bornyl acetate		196.29	6, 82	0.982	1.4626	27	224	84	v sl s aq; s alc, eth
b247	*N*-Bromoacetamide	$CH_3CON(Br)H$	137.96	2, 181			102–105			sl s aq; v s eth
b248	*p*-Bromoacetanilide	$BrC_6H_4NHCOCH_3$	214.06	12, 642	1.717		168			s alc, bz, chl, EtOAc
b249	Bromoacetic acid	$BrCH_2COOH$	138.95	2, 213	1.934_4^{50}	1.4804^{50}	50	208	>110	v s aq, alc
b250	Bromoacetonitrile	$BrCH_2CN$	119.95	2, 216	1.722	1.4800^{20}		62^{24mm}	>110	
b251	2-Bromoacetophenone	$C_6H_5COCH_2Br$	199.05	7, 283	1.647_4^{20}		50	135^{18mm}	>110	v s alc, bz, chl, eth
b253	*p*-Bromoacetophenone	$BrC_6H_4COCH_3$	199.05	7, 283	1.647		54	255	>110	s alc, bz, CS_2, HOAc PE
b254	Bromoacetyl bromide	$BrCH_2COBr$	201.86	2, 215	2.317_{22}^{22}	1.5480^{20}		150	none	dec aq, alc
b255	Bromoacetyl chloride	$BrCH_2COCl$	157.40	2, 215	1.908	1.4960^{20}		128	none	dec aq, alc
b256	2-Bromoaniline	$BrC_6H_4NH_2$	172.03	12, 631	1.578_4^{20}	1.6223^{20}	31	229	>110	i aq; s alc, eth
b257	3-Bromoaniline	$BrC_6H_4NH_2$	172.03	12, 633	1.580_4^{20}	1.6250^{20}	16.8	251	>110	sl s aq; s alc, eth
b258	4-Bromoaniline	$BrC_6H_4NH_2$	172.03	12, 636	1.4970_4^{100}		66.3			i aq; v s alc, eth
b259	2-Bromoanisole	$BrC_6H_4OCH_3$	187.04	6, 197	1.502	1.5740^{20}	2	223	96	
b260	4-Bromoanisole	$BrC_6H_4OCH_3$	187.04	6, 199	1.494	1.5640^{20}	9–10	223	94	
b261	3-Bromobenzaldehyde	BrC_6H_4CHO	185.03	7, 238	1.587	1.5935^{20}		230	96	i aq; v s alc, eth
b262	Bromobenzene	C_6H_5Br	157.01	5, 206	1.4952_4^{20}	1.5602^{20}	−30.6	156	51	0.045 aq[30]; 10.4 alc[25]; 71.6 eth[25]; misc bz, chl, PE

b263	Bromobenzene-d_5	C_6D_5Br	162.06		1.539	1.5585^{20}		53^{23mm}	51	
b264	4-Bromobenzene-sulfonyl chloride	$BrC_6H_4SO_2Cl$	255.52	11, 57			74.5	153^{15mm}		i aq; s alc (dec); v s eth
b265	2-Bromobenzoic acid	BrC_6H_4COOH	201.02	9, 347			148–150			
b266	4-Bromobenzoic acid	BrC_6H_4COOH	201.02	9, 351	1.929_4^{25}		251–253			0.18 aq^{25}; s alc, eth
b267	4-Bromobenzo-phenone	$BrC_6H_4COC_6H_5$	261.12	7, 422				82	350	i alc; sl s bz, eth
b268	2-Bromobenzotri-fluoride	$BrC_6H_4CF_3$	225.01		1.652^{20}	1.4820^{20}		168	51	
b269	3-Bromobenzotri-fluoride	$BrC_6H_4CF_3$	225.01		1.613	1.4730^{20}		152	43	
b270	3-Bromobenzoyl chloride	BrC_6H_4COCl	219.47	9, 350	1.662	1.5965^{20}		$75^{0.5mm}$	107	
b271	4-Bromobenzyl bromide	$BrC_6H_4CH_2Br$	249.94	5, 308		1.6193^{20}	61	124^{12mm}	>110	s aq, alc, bz, eth, CS_2, HOAc
b272	α-Bromobenzyl cyanide	$C_6H_5CH(Br)CN$	196.05		1.539_4^{29}	1.5696^{20}	29	242 dec	>110	sl s aq; v s alc, acet, eth. A war gas.
b273	4-Bromobiphenyl	$BrC_6H_4C_6H_5$	233.11	5, 580	0.9327_4^{25}		90–92	310		i aq; s alc, bz, eth
b274	1-Bromobutane	$CH_3CH_2CH_2CH_2Br$	137.02	1, 119	1.2686_4^{25}	1.4374^{25}	−112.4	101.6	18	i aq; s alc, bz, eth
b275	2-Bromobutane	$CH_3CH_2CHBrCH_3$	137.02	1, 119	1.2585^{20}	1.4360^{20}	−112.7	91.4	21	<0.1 aq; v s alc, eth
b276	1-Bromo-2-butene	$CH_3CH{=}CHCH_2Br$	135.01	1, 205	1.312	1.4765^{20}		99	11	
b277	2-Bromo-2-butene	$CH_3CH{=}C(Br)CH_3$	135.01	1, 205	1.328	1.4590^{20}		90^{740mm}	1	Mixture of *cis*, *trans*
b278	4-Bromo-1-butene	$BrCH_2CH_2CH{=}CH_2$	135.01	1[1], 84	1.3230_4^{20}	1.4608^{20}		100	9	i aq; s alc, eth
b279	4-Bromobutyl acetate	$CH_3CO_2(CH_2)_4Br$	195.06	2[3], 39	1.348	1.4600^{20}		93^{12mm}	109	
b280	1-Bromo-4-*tert*-butyl-benzene	$(CH_3)3CC_6H_4Br$	213.12	5, 416	1.229	1.5330^{20}	15–16	81^{2mm}	97	

Bromal, t199
Bromoacetaldehyde diethyl acetal, b317
Bromoanisoles, b357, b358, b359

p-Bromobenzenethiol, b428
4-Bromobenzyl cyanide, b397

exo-2-Bromobicyclo[2.2.1]heptane, b383
Bromobutanedioic acid, b421



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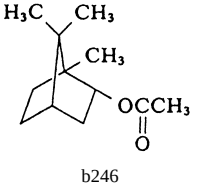


b246

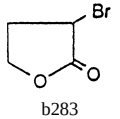
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b281	4-Bromobutyl phenyl ether	$C_6H_5O(CH_2)_4Br$	229.12	6^2, 82			41–43	156^{18mm}	>110	
b282	2-Bromobutyric acid	$CH_3CH_2CH(Br)COOH$	167.00	2, 281	1.5669_{20}^{20}	1.4720^{20}	−4	103^{10mm}	>110	6.7 aq; s alc, eth
b283	α-Bromo-γ-butyro-lactone		164.99		1.990^{20}	1.5080^{20}		138^{6mm}	>110	
b284	[1*R-endo*]-(+)-3-Bromocamphor		231.14	7, 120	1.449		75–78	244		15 alc; 200 chl; 62 eth; s olive oil
b285	1-Bromocarbonyl-1-methylethyl acetate	$CH_3CO_2C(CH_3)_2COBr$	209.05		1.431	1.4570^{20}		77^{12mm}	110	
b286	2-Bromo-4′-chloro-acetophenone	$ClC_6H_4COCH_2Br$	233.50							
b287	2-Bromochloro-benzene	BrC_6H_4Cl	191.46	5, 209	1.6382_4^{25}	1.5789^{25}		204	79	i aq; v s bz
b288	3-Bromochloro-benzene	BrC_6H_4Cl	191.46	5, 209	1.6302_4^{20}	1.5770^{20}	−21	196	80	i aq; v s alc, bz, eth
b296	4-Bromochloro-benzene	BrC_6H_4Cl	191.46	5, 209	1.576_4^{71}	1.5531^{70}	66	196		0.1 aq; misc MeOH, eth
b297	3-Bromo-4-chloro-benzotrifluoride	$Br(Cl)C_6H_3CF_3$	259.46	5^3, 715	1.726	1.4990^{20}	−22	190	94	
b298	1-Bromo-4-chloro-butane	$ClCH_2CH_2CH_2CH_2Br$	171.47	5^3, 294	1.488	1.4875^{20}		82^{30mm}	60	i aq; s alc, chl, eth
b299	4′-Bromo-4-chloro-butyrophenone	$BrC_6H_4CO(CH_2)_3Cl$	261.55				36–38		>110	
b300	4-Bromo-6-chloro-*o*-cresol	$Br(Cl)C_6H_2(OH)CH_3$	221.49	6, 360			45–47		>110	
b301	Bromochlorodifluoro-methane	$Br(Cl)CF_2$	165.36		6.579 g/L		−160	−3.7		
b302	3-Bromo-1-chloro-5,5-dimethyl-hydantoin		241.48				160–164			
b303	1-Bromo-2-chloro-ethane	$ClCH_2CH_2Br$	143.41	1, 89	1.7392_4^{20}	1.4917^{20}	−18.4	106.6		0.7 aq; misc org solv
b303a	Bromochlorofluoro-methane	Br(Cl)CHF	149.37		1.9771^0	1.4144^{55}	−115	36		

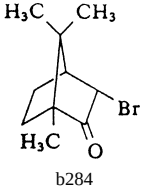
b304	7-Bromo-5-chloro-8-hydroxyquinoline		258.51	21[1], 222			177–179			
b305	Bromochloromethane	$ClCH_2Br$	129.38	1, 67	1.923_4^{25}	1.480^{25}	−88	68		0.9 aq; misc MeOH, eth
b306	1-Bromo-3-chloro-2-methylpropane	$ClCH_2CH(CH_3)CH_2Br$	171.47	1[3], 324	1.467	1.4809^{20}		154	>110	
b307	1-Bromo-3-chloro-propane	$ClCH_2CH_2CH_2Br$	157.44	1, 109	1.492	1.4851^{20}	< −50	143.5		0.1 aq; misc org solv
b308	2-Bromo-2-chloro-1,1,1-trifluoroethane	$BrCH(Cl)CF_3$	197.39	1[4] 156	1.8636^{25}	1.3691^{20}		50.2	none	
b309	2-Bromocinnam-aldehyde	$C_6H_4CH{=}C(Br)CHO$	211.06	7, 358			66–68			
b310	Bromocycloheptane	$Br(C_7H_{13})$	177.09	5, 29	1.2887_4^{22}	1.5052^{20}		72^{10mm}	68	i aq; v s chl, eth
b311	Bromocyclohexane	$Br(C_6H_{11})$	163.06	5, 24	1.3264_4^{15}	1.4956^{15}		165.8	62	0.1 aq; 10 MeOH; 71 eth
b312	3-Bromocyclohexene		161.04	5[2], 40	1.3890_4^{20}	1.5292^{20}		65^{15mm}	54	
b313	Bromocyclopentane	$Br(C_5H_9)$	149.04	5, 19	1.3900_4^{20}	1.4881^{20}		137–139	35	
b314	Bromocyclopropane	$Br(C_3H_5)$	120.98		1.510	1.4605^{29}		69	−6	
b315	1-Bromodecane	$CH_3(CH_2)_9Br$	221.18	1[2], 130	1.0658_4^{20}	1.4560^{20}	−30	238–240	94	i aq; v s chl, eth
b316	Bromodichloro-methane	$BrCHCl_2$	163.83	1, 67	1.980^{20}	1.4967^{20}	−55	87	none	sl s aq; misc org solv
b317	2-Bromo-1,1-di-ethoxyethane	$BrCH_2CH(OC_2H_5)_2$	197.08	1, 625	1.310	1.4385^{20}		67^{18mm}	51	s hot alc
b318	4-Bromo-1,2-di-methoxybenzene	$BrC_6H_3(OCH_3)_2$	217.07	6, 784	1.702	1.5743^{20}	256	109		
b319	2-Bromo-1,1-di-methoxyethane	$BrCH_2CH(OCH_3)_2$	169.02	1, 624	1.430	1.4450^{20}		150	53	

2-Bromo-*p*-cumene, b351

β-Bromocumene, b350



b283



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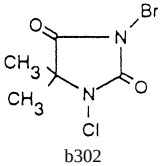

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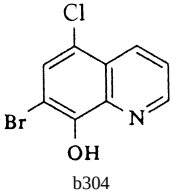

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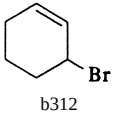


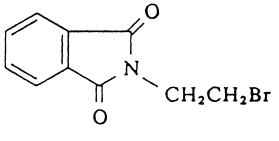
b312

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b320	1-Bromo-2,2-dimethoxypropane	$CH_3C(OCH_3)_2CH_2Br$	185.05		1.355	1.4475^{20}		87^{80mm}	40	
b321	4-Bromo-2,6-dimethylphenol	$BrC_6H_2(CH_3)_2OH$	201.07	6, 485			79–81			
b322	3-Bromo-2,2-dimethyl-1-propanol	$BrCH_2C(CH_3)_2CH_2OH$	167.05	1^1, 201	1.358	1.4794^{20}		184–187	75	
b323	2-Bromo-4,6-dinitroaniline	$BrC_6H_2(NO_2)_2NH_2$	262.03	12, 761			154	subl		v s hot alc, hot acet
b324	1-Bromo-2,4-dinitrobenzene	$BrC_6H_3(NO_2)_2$	247.01				71–73			
b325	4-Bromodiphenyl ether	$BrC_6H_4OC_6H_5$	249.11	6^1, 105	1.423	1.6070^{20}	18	305	>110	
b326	1-Bromodiphenylmethane	$C_6H_5CH(Br)C_6H_5$	247.14	5, 592			40–42	184^{20mm}	>110	
b327	1-Bromododecane	$CH_3(CH_2)_{11}Br$	249.24	1^2, 133	1.038	1.4580^{20}	−11	135^{6mm}	>110	0.1 aq; s alc, eth
b328	1-Bromo-2,3-epoxypropane		136.98	17, 9	1.601^{20}	1.4820^{20}	−40	134–136	56	i aq; sl s alc; s eth
b329	Bromoethane	CH_3CH_2Br	108.97	1, 88	1.4612_4^{20}	1.4242^{20}	−119	38.2	−23	0.91 aq^{20}; misc alc, chl, eth
b330	2-Bromoethanesulfonic acid, sodium salt	$BrCH_2CH_2SO_2^-\ Na^+$	211.02	4, 7			283 dec			
b331	2-Bromoethanol	$BrCH_2CH_2OH$	124.98	1, 338	1.7629_4^{20}	1.4936^{20}		57^{20mm}	>110	misc aq; s org solv except PE
b332	2-Bromoethyl acetate	$CH_3CO_2CH_2CH_2Br$	167.01	2^1, 57	1.514_4^{20}	1.4547^{20}	−13.8	159	71	v s aq; misc alc, eth
b333	2-Bromoethylamine HBr	$BrCH_2CH_2NH_2 \cdot HBr$	204.90	4, 134			172–174			v s aq, alc
b334	(1-Bromoethyl)-benzene	$C_6H_5CH(CH_3)Br$	185.07	5, 355	1.356	1.5600^{20}		94^{16mm}	81	
b334a	(2-Bromoethyl)-benzene	$C_6H_5CH_2CH_2Br$	185.07	5, 355	1.355	1.5560^{20}		221	89	
b335	1-Bromo-2-ethylbenzene	$BrC_6H_4CH_2CH_3$	185.07	5, 355	1.338	1.5490^{20}		194^{16mm}	71	
b336	Bromoethylene	$H_2C{=}CHBr$	106.95	1, 188	1.493^{20}	1.4380^{20}	−139	15.8	none	i aq; misc alc, eth

b337	2-Bromoethyl ethyl ether	$BrCH_2CH_2OCH_2CH_3$	153.02	1, 338	1.3572_4^{20}	1.4450^{20}		150	21	sl s aq; misc alc, eth
b338	2-Bromoethyl phenyl ether	$BrCH_2CH_2OC_6H_5$	201.07	6, 142			34	144^{40mm}	65	i sq; v s alc, eth
b339	*N*-(2-Bromoethyl)-phthalimide		254.09	21, 461			81–84			s hot aq; v s eth
b340	1-Bromo-2-fluoro-benzene	BrC_6H_4F	175.01		1.601	1.5337^{20}		156	43	
b341	1-Bromo-3-fluoro-benzene	BrC_6H_4F	175.01		1.567	1.5257^{20}		150	38	
b342	1-Bromo-4-fluoro-benzene	BrC_6H_4F	175.01	5, 209	1.593^{15}	1.5310^{15}	−17.4	152	60	
b343	1-Bromoheptane	$H(CH_2)_7Br$	179.11	1, 155	1.1384_4^{20}	1.4505^{20}	−58	180	60	i aq; v s alc, eth
b344	2-Bromoheptane	$H(CH_2)_5CH(Br)CH_3$	179.11	1, 155	1.142	1.4470^{20}		66^{21mm}	47	
b345	1-Bromohexadecane	$H(CH_2)_{16}Br$	305.35	1^2, 138	0.9991	1.4618^{20}	17.8	336	177	i aq; misc org solv
b346	1-Bromohexane	$H(CH_2)_6Br$	165.08	1, 144	1.1763_4^{20}	1.4475^{20}	−85	154–158	57	i aq; misc alc, eth
b347	**DL**-2-Bromohexanoic acid	$CH_3(CH_2)_3CH(Br)COOH$	195.06	2, 325	1.370	1.4720^{20}		138^{18mm}	>110	s alc, eth
b348	5-Bromoisatin		226.03	21, 453			251–253			
b350	(2-Bromoisopropyl)-benzene	$C_6H_5CH(CH_3)CH_2Br$	199.10	5^1, 191	1.316	1.5480^{20}		108^{18mm}	91	
b351	2-Bromo-4-isopropyl-1-methylbenzene	$CH_3(Br)C_6H_3CH(CH_3)_2$	213.0		1.253_{25}^{25}	1.535^{25}	−20	120		i aq; 50 MeOH; misc org solvents
b352	Bromomaleic anhydride		176.96	17, 435	1.905	1.5400^{20}		215	>110	
b353	2-Bromomesitylene	$1,3,5\text{-}(CH_3)_3C_6H_2Br$	199.10	5, 408	1.301	1.5520^{20}	2	255	96	
b354	Bromomethane	CH_3Br	94.94	1, 67	1.732_0^0	1.4234^{10}	−94	3.56	none	0.1 aq; s alc, chl, eth
b355	4-Bromomandelic acid	$BrC_6H_4CH(OH)COOH$	231.05	10, 210			117–118			sl s aq

4-Bromodiphenyl ether, b295
Bromoethene, b336
Bromoform, t204
2-Bromomesitylene, b436



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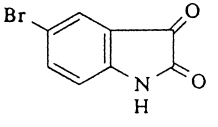

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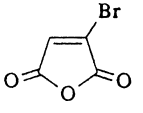


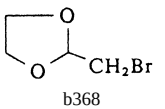
b352

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

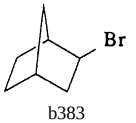
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b356	5-Bromo-2-methoxy-benzaldehyde	$BrC_6H_3(OCH_3)CHO$	215.05	8, 55			116–119			
b357	2-Bromo-1-methoxy-benzene	$BrC_6H_4OCH_3$	187.04	6, 197	1.5018_4^{20}	1.5737^{20}	2	223	96	i aq; v s alc, eth
b358	3-Bromo-1-methoxy-benzene	$BrC_6H_4OCH_3$	187.04	6, 198	1.477	1.5635^{20}	211	93		i aq; s alc, eth
b359	4-Bromo-1-methoxy-benzene	$BrC_6H_4OCH_3$	187.04	6, 199	1.4564_4^{20}	1.5630^{20}	10	223	94	sl s aq; v s alc, eth
b360	4-Bromo-2-methyl-aniline	$CH_3(Br)C_6H_3NH_2$	186.06	12, 838			57–59	240	>110	sl s aq; v s alc
b361	1-Bromo-3-methyl-benzyl alcohol	$BrC_6H_4CH(CH_3)OH$	201.07	6^2, 447	1.460		36–38	121^{7mm}	63	
b362	1-Bromo-3-methyl-butane	$(CH_3)_2CHCH_2CH_2Br$	151.05	1, 136	1.210_4^{15}	1.4409^{20}	−112	119.7	32	0.02 aq; misc alc, eth
b363	2-Bromo-2-methyl-butane	$C_2H_5C(CH_3)_2Br$	151.05	1, 136	1.182	1.4423^{20}		107^{735mm}	5	
b364	2-Bromo-3-methyl-butanoic acid	$(CH_3)_2CHCH(Br)COOH$	181.04	2, 317			44	126^{20mm}	107	sl s aq; s alc, eth
b365	4-Bromo-2-methyl-2-butene	$BrCH_2C{=}C(CH_3)_2$	149.04	1^2, 189	1.293	1.4898^{20}		60^{60mm}	32	
b366	(Bromomethyl)chloro-dimethylsilane	$BrCH_2Si(CH_3)_2Cl$	187.5	4^4, 4024	1.375	1.4650^{20}		130^{740mm}	41	
b367	(Bromomethyl)cyclo-hexane	$(C_6H_{11})CH_2Br$	177.09	5^2, 18	1.269	1.4907^{20}		77^{26mm}	57	
b368	2-Bromomethyl-1,3-dioxalane		167.01	19^2, 8	1.613	1.4817^{20}		82^{27mm}	62	
b369	Bromomethyl methyl ether	$BrCH_2OCH_3$	124.97	1, 582	1.531	1.4550^{20}		87	26	
b370	1-Bromo-2-methyl-naphthalene	$Br(C_{10}H_6)CH_3$	221.10	5, 568	1.418	1.6486^{20}		296	>110	
b371	1-Bromo-2-methyl-propane	$(CH_3)_2CHCH_2Br$	137.03	1, 126	1.2641^{20}	1.4362^{20}	−119	91.5	18	0.06 aq; misc alc, eth

b372	2-Bromo-2-methyl-propane	$(CH_3)_3CBr$	137.03	1, 127	1.2125_4^{25}	1.425^{25}	−16.2	73.1	18	i aq; misc org solv
b373	2-Bromo-2-methyl-propanoic acid	$BrC(CH_3)_2COOH$	167.01	2, 295	1.52		48–49	200	>110	sl s aq; s alc, eth; dec by hot aq
b374	2-Bromo-2-methyl-propionyl bromide	$(CH_3)_2C(Br)COBr$	229.91	2, 297	1.860	1.5064^{24}		164	110	
b375	2-Bromo-2-methyl-propiophenone	$C_6H_5CO(CH_3)_2Br$	227.11	7, 316	1.350	1.5561^{20}		148^{30mm}	>112	
b376	1-Bromonaphthalene	$(C_{10}H_7)Br$	207.07	5, 547	1.4834_4^{20}	1.6580^{20}	−1.8	281	>110	misc alc, bz, chl, eth
b377	1-Bromo-1-naphthol	$BrC_{10}H_6OH$	233.07	6, 650			78	130 dec		i aq; s alc, bz, eth
b378	1-Bromo-2-naphthol	$BrC_{10}H_6OH$	223.07	6, 650			78–81			
b379	1-Bromo-2-nitro-benzene	$BrC_6H_4NO_2$	202.01	5^1, 247	1.6245_4^{80}		43	261	110	v s alc; s bz, eth
b380	5-Bromo-2-nitrobenzo-trifluoride	$O_2N(Br)C_6H_3CF_3$	270.02	5^3, 755	1.7992^{25}	1.5180^{25}	33–35	100^{5mm}	>110	
b381	2-Bromo-2-nitro-1,3-propanediol	$(HOCH_2)_2C(Br)NO_2$	199.99	1, 476			120–122			s aq, alc, EtOAc; sl s bz, acet, chl, eth
b382	1-Bromononane	$H(CH_2)_9Br$	207.16	1^1, 63	1.084	1.4540^{20}		201	90	i aq; s chl, eth
b383	*exo*-2-Bromo-norbor-nane		175.07		1.363	1.5148^{20}		82^{29mm}	60	
b384	1-Bromooctadecane	$H(CH_2)_{18}Br$	333.41	1^1, 69	0.976		23	216^{12mm}	>110	i aq; s alc, eth
b385	1-Bromooctane	$H(CH_2)_8Br$	193.13	1, 160	1.108_4^{25}	1.4518^{25}	−55	201	78	i aq; misc alc, eth
b386	Bromopentafluoro-benzene	BrC_6F_5	246.97		1.947^{20}	1.4490^{20}	−31	137	87	
b387	1-Bromopentane	$H(CH_2)_5Br$	151.05	1, 131	1.2237_4^{15}	1.4444^{20}	−88	129.6	31	i aq; s alc; misc eth
b388	2-Bromopentane	$CH_3CH_2CH_2CH(Br)CH_3$	151.05	1, 131	1.2039_4^{20}	1.4403^{20}		117	20	
b389	3-Bromopentane	$C_2H_5CH(Br)C_2H_5$	151.05	1^1, 43	1.216	1.4445^{20}		119	18	
b390	5-Bromopentyl acetate	$CH_3CO_2(CH_2)_5Br$	209.09	2^3, 249	1.255	1.4620^{20}		110^{15mm}	>110	

(Bromomethyl)benzene, b85
4-Bromo-1-methylbenzene, b431
2-Bromo-2-methylpropanoyl bromide, b374
α-Bromo-*p*-nitrotoluene, n44



b368



b383

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

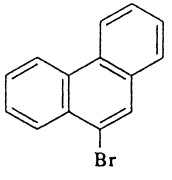
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b391	9-Bromophenanthrene		257.14	5, 671	1.409_4^{101}		54–58	190^{2mm}	>110	i aq; s alc, eth
b392	2-Bromophenol	BrC_6H_4OH	173.01	6, 197	1.492	1.5892^{20}	6	194	42	s aq; misc chl, eth
b393	3-Bromophenol	BrC_6H_4OH	173.01	6, 198			32	236	>110	
b394	4-Bromophenol	BrC_6H_4OH	173.01	6, 198	1.5875^{80}		64	238		14 aq; v s alc, chl
b395	1-(4-Bromophenoxy)-1-ethoxyethane	$CH_3CH(OC_6H_4Br)OC_2H_5$	245.12		1.348	1.5229^{20}		125^{8mm}	106	
b396	4-Bromophenylacetic acid	$BrC_6H_4CH_2COOH$	215.05	9, 451			119			sl s aq; v s alc, eth
b397	4-Bromophenylacetonitrile	$BrC_6H_4CH_2CN$	196.05	9, 451			47–49		>110	i aq; sl s alc; v s bz
b398	4-Bromophenyl phenyl ether	$BrC_6H_4OC_6H_5$	249.11	6[1], 105	1.423	1.6070^{20}	18	305	>110	
b399	1-Bromo-3-phenylpropane	$BrC_6H_4CH_2CH_2CH_2Br$	199.10	5, 391	1.310	1.5450^{20}		220	101	
b400	1-Bromopropane	$CH_3CH_2CH_2Br$	122.99	1, 108	1.3597^{15}	1.4370^{15}	−110.1	71.0		0.23 aq[30]; misc alc
b401	2-Bromopropane	$CH_3CH(Br)CH_3$	123.99	1, 108	1.3222^{15}	1.4285^{15}	−89.0	59.5	19	0.3 aq[18]; misc alc, bz, chl, eth
b402	3-Bromo-1-propanol	$BrCH_2CH_2CH_2OH$	139.00	1, 356	1.5374_4^{20}	1.4858^{20}		62^{5mm}	93	s aq; misc alc, eth
b403	1-Bromo-2-propanone	CH_3OCH_2Br	136.98	Merck: 12, 1422	1.634^{23}	1.4697^{15}	−36.5	137		v sl s aq; s alc, acet
b404	1-Bromo-1-propene	$CH_3CH{=}CHBr$	120.98	1, 200	1.4133_4^{20}	1.4538^{20}	−116	70	−6	i aq
b405	2-Bromo-2-propene	$CH_3C(Br){=}CH_2$	120.98	1, 200	1.362_4^{20}	1.4425^{20}	−125	47–49	4	
b406	2-Bromopropionic acid	$CH_3CH(Br)COOH$	152.98	2, 254	1.7000^{20}	1.4750^{20}	25.7	203	100	v s aq, alc, bz, chl, eth
b407	3-Bromopropionic acid	$BrCH_2CH_2COOH$	152.98	2, 256	1.480		62.5		65	s aq, alc, bz, chl, eth
b408	3-Bromopropionitrile	$BrCH_2CH_2CN$	133.98	2[2], 231	1.6152_4^{20}	1.4800^{20}		78^{10mm}	98	v s alc, eth
b409	2-Bromopropionyl bromide	$CH_3CH(Br)COBr$	215.88	2, 256	2.061	1.5182^{20}		50^{10mm}	>110	
b410	2-Bromopropionyl chloride	$CH_3CH(Br)COCl$	171.43	2, 256	1.700^{11}	1.4800^{20}		133	51	d aq; s chl, eth
b411	3-Bromopropionyl chloride	$CH_3CH(Br)COCl$	171.43	2[2], 231	1.701	1.4968^{20}		57^{17mm}	79	
b412	2-Bromopropiophenone	$C_6H_5COCH(Br)CH_3$	213.08	7, 302	1.430_4^{20}	1.5715^{20}		250	>110	s alc, bz, eth, acet

b413	3-Bromopropyl phenyl ether	$C_6H_5OCH_2CH_2CH_2Br$	215.10	6, 142	1.365	1.5464^{20}	10–11	134^{14mm}	96	
b414	3-Bromopropyltrichlorosilane	$Br(CH_2)_3SiCl_3$	256.44		1.605	1.4900^{20}		202–204	76	
b415	3-Bromopropyne	$BrCH_2C{\equiv}CH$	118.97	1, 248	1.335	1.4905^{20}		88–90	18	
b416	2-Bromopyridine	$Br(C_5H_4N)$	158.00	20, 233	1.657^{18}	1.5720^{20}		194	54	i aq; s org solv
b417	3-Bromopyridine	$Br(C_5H_4N)$	158.00	20, 233	1.645^{0}_{4}	1.5695^{20}	142–143	173	51	s aq; v s alc, eth
b418	3-Bromoquinoline		208.06	20, 363	1.533	1.6640^{20}	15	276	>110	s HOAc
b419	5-Bromosalicylic acid	$Br(HO)C_6H_3COOH$	217.02	10, 107			166			0.3 aq^{80}; 85 alc^{25}; 70 eth^{25}
b420	β-Bromostyrene	$C_6H_5CH{=}CHBr$	183.05	5, 477	1.422^{20}_{4}	1.6066^{20}	7	112^{20mm}	79	i aq; misc alc, eth
b421	(±)-Bromosuccinic acid	$HOOCH_2CH(Br)COOH$	196.99	2, 621	2.073		161			18 aq; s alc, acet, eth
b422	*N*-Bromosuccinimide		177.99	21, 380	2.098		173 sl dec			1.5 aq^{25}; 14.4 $acet^{25}$; 3.1 $HOAc^{25}$
b423	1-Bromotetradecane	$H(CH_2)_{14}Br$	277.30	1^2, 136	1.0124^{25}_{4}	1.4600^{20}	6	178^{20mm}	>110	s alc; v s chl; misc bz, acet
b424	3-Bromotetrahydro-2-methyl-2*H*-pyran		179.06	17^3, 75	1.366	1.4830^{20}		61^{17mm}	57	
b425	3-Bromothioanisole	$BrC_6H_4SCH_3$	203.11	6, 330			38–40		>110	
b426	2-Bromothiophene	$Br(C_5H_3S)$	163.04	17, 33	1.684^{20}_{4}	1.5860^{20}		151	60	v s acet, eth
b427	3-Bromothiophene	$Br(C_5H_3S)$	163.04		1.740	1.5910^{20}		150	56	
b428	4-Bromothiophenol	BrC_6H_4SH	189.08	6, 330			76	239		
b429	2-Bromotoluene	$BrC_6H_4CH_3$	171.04	5, 304	1.422^{25}_{25}	1.552^{25}	−26	181	78	0.1 aq; misc alc, bz, chl, eth

β-Bromophenitole, b338
3-Bromopropene, a79

(3-Bromopropyl)benzene, b338
3-Bromopropylene, a79

5-Bromopseudocumene, b435
α-Bromotoluene, b85



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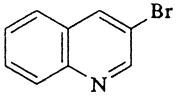

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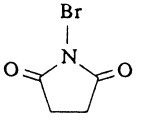

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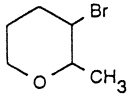


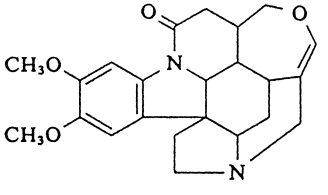
b424

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b430	3-Bromotoluene	$BrC_6H_4CH_3$	171.04	5, 305	1.4099^{20}	1.5517^{20}	−39.8	183.7	60	s alc, bz, eth
b431	4-Bromotoluene	$BrC_6H_4CH_3$	171.04	5, 305	1.3959^{35}_{35}	1.5490	28.5	184.5	85	s alc, bz, eth
b432	Bromotrichloro-methane	$BrCCl_3$	198.28	1, 67	1.997^{25}_{25}	1.5063^{20}	−6	104–105		misc org solv
b433	1-Bromotridecane	$H(CH_2)_{13}Br$	263.27	1^2, 134	1.0262^{20}_{4}	1.4592^{20}	7	150^{10mm}	>110	v s chl
b434	Bromotrifluoro-methane	$BrCF_3$	148.91	1^3, 83	6.087 g/L		−168 to −172	−57.8		v s chl
b435	5-Bromo-1,2,4-tri-methylbenzene	$BrC_6H_2(CH_3)_3$	199.10	5, 403			73	235		i aq; s alc
b436	2-Bromo-1,3,5-tri-methylbenzene	$BrC_6H_2(CH_3)_3$	199.10	5, 408	1.301	1.5511^{20}	2	225	96	i aq; s bz; v s eth
b437	Bromotrimethyl-germane	$(CH_3)_3GeBr$	197.60		1.544^{18}	1.4705^{20}	−25	113.7	37	
b438	Bromotrimethylsilane	$(CH_3)_3SiBr$	153.10		1.160	1.4140^{20}		79	32	
b439	Bromotriphenyl-ethylene	$(C_6H_5)_2C{=}C(Br)C_6H_5$	335.22	5, 722			115–117			
b440	Bromotriphenyl-methane	$(C_6H_5)_3CBr$	323.24	5, 704			152–154	230^{15mm}		
b441	1-Bromoundecane	$CH_3(CH_2)_{10}Br$	235.22	1^2, 132	1.954	1.4563^{20}	−9	138^{18mm}	>110	
b442	11-Bromoundecanoic acid	$Br(CH_2)_{10}COOH$	265.20	2^2, 315			51	174^{2mm}	>110	i aq; v s alc
b443	α-Bromo-1,2-xylene	$BrCH_2C_6H_3CH_3$	185.07	5, 365	1.381^{23}	1.381^{20}	21	224	82	s alc, eth
b444	α-Bromo-1,3-xylene	$BrCH_2C_6H_3CH_3$	185.07	5, 374	1.370^{23}	1.5560^{20}		185^{340mm}	82	s alc, eth
b445	2-Bromo-1,4-xylene	$BrCH_2C_6H_3CH_3$	185.07	5, 385	1.340	1.5505^{20}	9–10	199–201	79	v s chl, hot ether
b446	4-Bromo-1,2-xylene	$BrCH_2C_6H_3CH_3$	185.07	5, 365	1.370^{15}_{15}	1.5560^{20}		215	80	v s alc, eth
b447	Brucine		394.45	27^2, 797			178			77 alc; 1 bz; 20 chl; 4 EtOAc
b448	1,2-Butadiene	$CH_3CH{=}C{=}CH_2$	54.09	1, 249	0.676^{10}	1.4205^{1}	−136.2	10.9		misc alc, eth
b449	1,3-Butadiene	$H_2C{=}CHCH{=}CH_2$	54.09	1, 249	2.211 g/L	1.4293^{-25}	−108.9	−4.4	−76	misc alc, eth
b450	Butadiene sulfone		118.15	17^3, 144			66		>110	
b451	1,3-Butadienyl acetate	$CH_3CO_2CH{=}CHCH{=}CH_2$	112.13	2^3, 295	0.945	1.4690^{20}		60^{40mm}	33	
b452	1,3-Butadiyne	$HC{\equiv}CC{\equiv}CH$	50.06	1^3, 1056	0.7364^{0}_{4}	1.4189^{5}	−36	10.3		v s eth; s acet, bz

b453	2-Butanamine	$CH_3CH_2CH(NH_2)CH_3$	73.14	4, 160	0.7308_4^{15}	1.3963^{15}	−104.5	66	−19	misc aq, alc
b454	Butane	$CH_3CH_2CH_2CH_3$	58.12	1, 118	0.6011^{0}	1.3562^{-13}	−138.3	−0.50	−60	1 vol aq dissolves 0.15 vol and 1 vol alc 18 vols at 17° and 770 mm; 1 vol ether or $CHCl_3$ dissolves 25 or 30 vols, resp.
b455	1,4-Butanediamine	$H_2NCH_2CH_2CH_2CH_2NH_2$	88.15	4, 264	0.877_4^{25}	1.4569^{20}	28	158–160	51	s aq
b456	Butanedinitrile	$NCCH_2CH_2CN$	80.09	2, 615	0.9867_4^{60}	1.4173^{60}	54.5	266	132	11.5 aq; s acet, chl, 1,4-dioxane; sl s bz
b457	1,2-Butanediol	$CH_3CH_2CH(OH)CH_2OH$	90.12	1, 477	1.006_0^{18}	1.4380^{20}		207.5	93	s aq, alc, acet
b457a	1,3-Butanediol	$CH_3CH(OH)CH_2CH_2OH$	90.12	1, 477	1.0053_{20}^{20}	1.441^{20}	< −50	207.5	121	s aq, alc, acet; 9 eth
b457b	1,4-Butanediol	$HOCH_2CH_2CH_2CH_2OH$	90.12	1, 478	1.016_4^{25}	1.4452^{20}	20	235	121	misc aq, alc, acet; 0.3 bz; 3.1 eth; 0.9 PE
b458	*meso*-2,3-Butanediol	$CH_3CH(OH)CH(OH)CH_3$	90.12	1, 479	0.9939_4^{25}	1.4324^{35}	25	182	85	misc aq, alc
b459	1,4-Butanediol dimethanesulfonate	$CH_3SO_2O(CH_2)_4OSO_2CH_3$	246.30	4^4, 19			114–117			2.4 $acet^{25}$; 0.1 alc^{25}
b460	1,3-Butanediol diacetate	$CH_3CO_2CH_2CH_2CH(CH_3)$-O_2CCH_3	174.20	2, 143	1.028	1.4199^{20}		99^{8mm}	85	
b461	1,4-Butanediol diacrylate	$(H_2C{=}CHCO_2CH_2CH_2$-$)_2$	198.22	2^4, 170	1.051	1.4560^{20}		$83^{0.3mm}$	>110	

Bromo-α,α,α-trifluorotoluene, b268, b269
3-Bromo-1,7,7-trimethylbicyclo[2.2.1]heptane-2-one, b284
4-Bromoveratrole, b318
4-Bromo-2,6-xylenol, b321
BSA, b230
BSTFA, b235
BTMSA, b231
Busulfan, b210
1,3-Butadiene diepoxide, d546
Butanal, b612
1-Butanamine, b509
Butanecarbaldehyde, p28
Butanedinitrile, s18
Butanedioic acid, s15
Butanedioic anhydride, s16
1,4-Butanediol diglycidyl ether, b185



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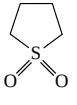


b450

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b462	1,3-Butanediol dimethacrylate	$H_2C{=}C(CH_3)CO_2CH_2CH_2$-$CH(CH_3)O_2CC(CH_3){=}CH_2$	226.28		1.010	1.4520^{20}		290	>110	
b463	1,4-Butanediol dimethacrylate	$[H_2C{=}C(CH_3)CO_2CH_2CH_2\text{-}]_2$	226.28	2^4, 1534	1.010	1.4560^{20}		134^{4mm}	>110	
b464	1,4-Butanediol divinyl ether	$(\text{-}CH_2CH_2OCH{=}CH_2)_2$	142.20	1^4, 2518	0.898	1.444^{20}	−8	64^{10mm}	62	
b465	1,4-Butanediol vinyl ether	$H_2C{=}CHO(CH_2)_4OH$	116.16	1^4, 2518	0.939	1.4440^{20}		95^{20}	85	
b466	2,3-Butanedione	$CH_3C(=O)C(=O)CH_3$	86.09	1, 769	0.990^{15}_{15}	1.3951^{20}		86	7	25 aq; misc alc, eth
b467	2,3-Butanedione monoxide	$CH_3C(=NOH)C(=O)CH_3$	101.11	1, 772			75–78	186		
b468	1,4-Butanedithiol	$HSCH_2CH_2CH_2CH_2SH$	122.25	1, 479	1.042	1.5290^{20}		106^{30mm}	70	i aq; v s alc
b468a	Butanenitrile	$CH_3CH_2CH_2CN$	69.11	2^2, 252	0.7936	1.4440^{20}	−112	117.6	24	3.3 aq; misc alc, eth
b469	1,2,3,4-Butanetetracarboxylic acid	$[\text{-}CH(COOH)CH_2COOH]_2$	234.16	2, 863			196			
b470	1-Butanethiol	$CH_3CH_2CH_2CH_2SH$	90.19	1, 370	0.8367^{25}_{4}	1.4430^{25}	−116	98.5	2	0.06 aq; v s alc, eth
b471	2-Butanethiol	$CH_3CH_2CH(SH)CH_3$	90.19	1, 373	0.8246^{25}_{4}	1.4338^{25}	−165	85.0	21	sl s aq; v s alc, eth
b472	1,2,4-Butanetriol	$HOCH_2CH_2CH(OH)CH_2OH$	106.12	1, 519	1.190^{20}	1.4748^{20}		191^{18mm}	167	v s aq, alc
b473	1-Butanol	$CH_3CH_2CH_2CH_2OH$	74.12	1, 367	0.8097^{20}_{4}	1.3993^{20}	−89.5	117.7	37	7.4 aq; misc alc, eth
b474	2-Butanol	$CH_3CH_2CH(OH)CH_3$	74.12	1, 371	0.8069^{20}_{4}	1.3972^{20}	−114.7	99.5	24	12.5 aq; misc alc, eth
b475	2-Butanone	$CH_3CH_2COCH_3$	72.11	1, 666	0.8054^{20}_{4}	1.3788^{20}	−86.7	79.6	−9	24 aq; misc alc, bz, eth
b476	2-Butanone oxime	$CH_3CH_2C(=NOH)CH_3$	87.12	1, 668	0.924	1.4420^{20}		60^{15mm}	60	
b477	1-Butene	$CH_3CH_2CH{=}CH_2$	56.11	1, 203	0.6255^{mp}_{4}	1.3962^{20}	−185.3	−6.5	−80	i aq; v s alc, eth
b478	*cis*-2-Butene	$CH_3CH{=}CHCH_3$	56.11	1^3, 728	0.6213	1.3931^{-25}	−139.3	3.7	−73	i aq; v s alc, eth
b479	*trans*-2-Butene	$CH_3CH{=}CHCH_3$	56.11	1, 205	0.6041	1.3848^{-25}	−105.8	0.9	−73	i aq; v s alc, eth
b480	*cis*-2-Butene-1,4-diol	$HOCH_2CH{=}CHCH_2OH$	88.11	1^2, 567	1.0700^{20}_{4}	1.4780^{20}	2	234	128	s aq; v s alc
b481	*trans*-2-Butene-1,4-diol	$HOCH_2CH{=}CHCH_2OH$	88.11	1^3, 2252	1.070^{20}_{4}	1.4755^{20}	25	132		v s aq, alc
b482	3-Butenenitrile	$H_2C{=}CHCH_2CN$	67.09	2, 408	0.8341^{20}_{4}	1.4060^{20}	−87	119	21	sl s aq; misc alc, eth
b483	*cis*-2-Butenoic acid	$CH_3CH{=}CHCOOH$	86.09	2, 412	1.0267^{20}_{4}	1.4483^{14}	14–15	168–169		v s aq; s alc
b484	*trans*-2-Butenoic acid	$CH_3CH{=}CHCOOH$	86.09	2, 408	0.9604^{80}_{4}	1.4248^{77}	72	185	87	55 aq; 52 EtOH; 53 acet; 37 toluene
b485	3-Butenoic acid	$H_2C{=}CHCH_2COOH$	86.09	2, 407	1.0091^{20}_{4}	1.4249^{20}	−39	163	65	s aq; misc alc, eth
b486	*cis*-2-Buten-1-ol	$CH_3CH{=}CHCH_2OH$	72.11	1, 442	0.8662^{20}_{4}	1.4342^{20}	−89.4	123.6	56	16.6 aq; misc alc

b487	*trans*-2-Buten-1-ol	$CH_3CH{=}CHCH_2OH$	72.11	1, 442	0.8524_4^{20}	1.4289^{20}	< −30	121.2	56	16.6 aq; misc alc
b488	3-Buten-2-one	$H_2C{=}CHCOCH_3$	70.09	1, 728	0.8636_4^{20}	1.4086^{20}		81.4	−6	v s aq, alc, acet, eth
b489	1-Buten-3-yne	$HC{\equiv}CCH{=}CH_2$	52.07	1^3, 1032	0.7095_4^{1}	1.4161		5.1		
b490	4-Butoxyaniline	$CH_3(CH_2)_3OC_6H_4NH_2$	165.24	13^2, 226	0.992	1.5543^{20}		149^{13mm}	>110	
b491	4-Butoxybenzoic acid	$CH_3(CH_2)_3OC_6H_4COOH$	194.23	10^2, 93			150			
b492	Butoxycarbonylmethyl butyl phthalate	2-$[CH_3(CH_2)_3O_2CCH_2O_2C]$-$C_6H_4CO_2(CH_2)_3CH_3$	336.39	9,*3*, 4187	1.100	1.4900^{20}		219^{5mm}	>110	
b493	2-Butoxyethanol	$CH_3(CH_2)_3OCH_2CH_2OH$	118.18	1^2, 519	0.9012_4^{20}	1.4198^{20}	−75	168	69	5 aq; s most org solv
b494	1-*tert*-Butoxy-2-ethoxyethane	$(CH_3)_3COCH_2CH_2OC_2H_5$	146.23	1^3, 2085	0.834	1.4015^{20}		148	33	
b495	2-(2-Butoxyethoxy)-ethanol	$HOCH_2CH_2OCH_2CH_2OC_4H_9$	162.23	1^2, 521	0.9536_{20}^{20}	1.4306^{20}	−68.1	230.4	100	misc aq, alc, bz, acet, CCl_4, PE
b496	2-(2-Butoxyethoxy)-ethyl acetate	$CH_3CO_2(CH_2CH_2O)_2CH_2$-$CH_2CH_2CH_3$	204.27	2^3, 308	0.978	1.4260^{20}		245	>110	
b497	2-Butoxyethyl acetate	$CH_3CO_2CH_2CH_2O(CH_2)_3CH_3$	160.22	2^3, 307	0.942	1.4136^{20}		192	76	
b498	2-*tert*-Butoxy-2-methoxyethane	$(CH_3)_3CO_2CH_2CH_2OCH_3$	132.20	1^3, 2084	0.840	1.3985^{20}		132	25	
b499	1-*tert*-Butoxy-2-propanol	$(CH_3)_3COCH_2CH(OH)CH_3$	132.10	1^3, 2148	0.874	1.4130^{20}		143–145	44	
b500	3-Butoxypropylamine	$CH_3(CH_2)_3O(CH_2)_3NH_2$	73.14	4^3, 739	0.853	1.4260^{20}		170	63	
b501	Butyl acetate	$C_4H_9O_2CH_3$	116.16	2, 130	0.8813_4^{20}	1.3941^{20}	−77/−78	126	22	0.43 aq; misc alc, eth; s most org solvents
b502	**DL**-*sec*-Butyl acetate	$CH_3CO_2CH(CH_3)C_2H_5$	116.16	2^2, 131	0.8748^{20}	1.3888^{20}	−99	112	31	0.62 aq; s alc, eth
b503	*tert*-Butyl acetate	$(CH_3)_3CO_2CCH_3$	116.16	2, 131	0.8665_4^{20}	1.3870^{20}		95.1	16	i aq; misc alc, eth
b504	*tert*-Butylacetic acid	$(CH_3)CCH_2COOH$	116.16	2, 337	0.912	1.4115^{20}	6–7	190		
b505	*tert*-Butyl acetoacetate	$(CH_3)_3COC(=O)CH_2$-$C(=O)CH_3$	158.20		0.954	1.4180^{20}			60	
b506	2-Butylacrolein	$(CH_3(CH_2)_3C(=CH_2)CHO$	112.17	1^4, 3482	0.843	1.4348^{20}		139	33	
b507	*N*-*tert*-Butylacrylamide	$H_2C{=}CHCONHC(CH_3)_3$	127.19	4^4, 664			128–129			
b507a	Butyl acrylate	$H_2{=}CHCO_2(CH_2)_3CH_3$	128.17	2^2, 388	0.894	1.4180^{20}	−64	145	39	0.14 aq^{20}
b508	*tert*-Butyl acrylate	$H_2C{=}CHCO_2C(CH_3)_3$	128.17	2^3, 1228	0.875	1.4108^{20}		63^{60mm}	17	
b509	Butylamine	$CH_3CH_2CH_2CH_2NH_2$	73.14	4, 156	0.7327_4^{25}	1.3992^{25}	−50/−49	77	−12	misc aq, alc, eth
b510	(±)-*sec*-Butylamine	$C_2H_5CH(NH_2)CH_3$	73.14	4, 160	0.724_4^{20}	1.3928^{20}	−104	63	−9	misc aq, alc
b511	*tert*-Butylamine	$(CH_3)_3CNH_2$	73.14	4, 173	0.6951_4^{20}	1.3788^{20}	−66	44	−9	misc aq, alc

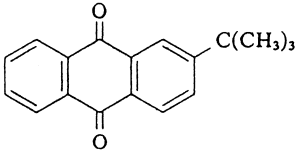
1,4-Butanediol dimethanesulfonate, b210
Butanoic acid, b614
Butanoic anhydride, b615
trans-2-Butenal, c306
Buten-4-carboxylic acid, p51
cis-2-Butenedioic acid, m1
2-Butene-1,1-diol diacetate, d28
trans-2-Buten-1-ol, c311
Butopyronoxyl, b550
Butoxybenzene, b591
1-Butoxybutane, d148
Butyl alcohols, b473, b474, m385

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b512	Butyl-4-aminobenzoate	$H_2NC_6H_4CO_2(CH_2)_3CH_3$	193.25	14^2, 249			57–59	174^{8mm}		v sl s aq; s dil acids, alc, chl, eth
b513	2-(*tert*-Butylamino)-ethanol	$(CH_3)_3CNHCH_2CH_2OH$	117.19				42–45	92^{25mm}	68	
b514	2-(*tert*-Butylamino)-ethyl methacrylate	$H_2C{=}C(CH_3)CO_2CH_2$-$CH_2NC(CH_3)_3$	185.27	4^4, 1509	0.914	1.4420^{20}		82^{10mm}	71	
b515	3-(*tert*-Butylamino)-1,2-propanediol	$(CH_3)_3CNHCH_2CH(OH)$-CH_2OH	147.22				70	92^{1mm}		
b516	2-Butylaniline	$CH_3(CH_2)_3C_6H_4NH_2$	149.24	12^2, 633	0.953	1.5380^{20}		123^{12mm}	108	
b517	2-*sec*-Butylaniline	$C_2H_5CH(CH_3)C_6H_4NH_2$	149.24	12^3, 2721	0.957	1.5410^{20}		122^{16mm}	>110	
b518	4-Butylaniline	$CH_3(CH_2)_3C_6H_4NH_2$	149.24	12^1, 503	0.945	1.5350^{20}		120^{15mm}	101	
b519	4-*sec*-Butylaniline	$C_2H_5CH(CH_3)C_6H_4NH_2$	149.24	12^2, 635	0.977	1.5370^{20}		245^{727mm}	107	
b520	2-*tert*-Butylanthraquinone		264.32				98–100			
b521	Butylbenzene	$CH_3CH_2CH_2CH_2C_6H_5$	134.22	5, 413	0.8604_4^{20}	1.4898^{20}	−88	183	71	misc alc, bz, eth
b522	*sec*-Butylbenzene	$C_2H_5CH(CH_3)C_6H_5$	134.22	5, 414	0.8608_4^{20}	1.4890^{20}	−82.7	173	52	misc alc, bz, eth
b523	*tert*-Butylbenzene	$(CH_3)_3CC_6H_5$	134.22	5, 415	0.8669_4^{20}	1.4923^{20}	−58.1	168.5	60	misc alc, bz, eth
b524	Butyl benzoate	$C_6H_5CO_2C_4H_9$	178.23	9, 112	1.0000^{20}	1.496	−22	250	106	i aq; s alc, eth
b525	2-Butylbenzofuran		174.25		0.987	1.5330^{20}			101	
b526	4-*tert*-Butylbenzoic acid	$(CH_3)_3CC_6H_4COOH$	178.23	9, 560	1.142_4^{20}		166.3			i aq; v s alc, bz
b527	4-*tert*-Butylbenzoyl chloride	$(CH_3)_3CC_6H_4COCl$	196.68		1.007	1.5364^{20}		135^{20mm}	87	
b528	*N*-(*tert*-Butyl)benzylamine	$C_6H_5CH_2NHC(CH_3)_3$	163.27	12, 1022	0.881	1.4968^{20}		80^{5mm}	80	
b529	*tert*-Butyl bromoacetate	$BrCH_2CO_2C(CH_3)_3$	195.06	2^1, 96	1.321	1.4450^{20}		50^{10mm}	49	
b530	Butyl 2-butoxy-2-hydroxyacetate	$CH_3(CH_2)_3OCH(OH)CO_2$-$(CH_2)_3CH_3$	204.27	3^4, 1497	0.996	1.4291^{20}		90^{40mm}	74	
b531	Butyl butyrate	$CH_3CH_2CH_2CCO_2C_4H_9$	144.22	2, 271	0.8692_4^{20}	1.4064^{20}	−91.5	166	49	i aq; misc alc, eth
b532	Butyl carbamate	$H_2NCO_2(CH_2)_3CH_3$	117.15				53–55		108	
b533	Butyl carbazate	$H_2NNHCO_2C(CH_3)_3$	132.16				39–42	$65^{0.03mm}$	91	
b534	4-*tert*-Butylcatechol	$(CH_3)_3C_6H_3$-1,2-$(OH)_2$	166.22		1.049_{25}^{60}		52–55	285	151	0.2 aq;[80] 240 eth;[25] s alc; v s acet

b535	*tert*-Butyl chloroacetate	$ClCH_2CO_2C(CH_3)_3$	150.61	2[3], 444	1.053	1.4230^{20}		49^{11mm}	46	
b536	4-*tert*-Butyl-1-chlorobenzene	$(CH_3)_3C_6H_4Cl$	158.67	5, 416	1.006	1.5108^{20}	23–25	217		
b537	*tert*-Butylchlorodiphenylsilane	$(CH_3)_3CSi(C_6H_5)_2Cl$	274.87		1.057	1.5675^{20}		$90^{0.02mm}$	>110	
b538	Butyl chloroformate	$ClCO_2C_4H_9$	136.58	3[2], 11	1.074_4^{25}	1.4114^{20}		142	25	d aq, alc; misc eth
b539	Butyl cyanoacetate	$NCCH_2CO_2C_4H_9$	141.17	2[1], 255	0.993	1.4254^{20}		115^{15mm}	87	
b540	*tert*-Butyl cyanoacetate	$NCCH_2CO_2C(CH_3)_3$	141.17		0.972	1.4200^{20}		108	91	
b541	Butylcyclohexane	$(C_6H_{11})_6C_4H_9$	140.27	5[1], 20	0.818	1.4400^{20}	−78	178–180	41	
b542	*tert*-Butylcyclohexane	$(C_6H_{11})C(CH_3)_3$	140.27	5[1], 20	0.831	1.4470^{20}		167	42	
b543	2-*tert*-Butylcyclohexanol	$(CH_3)_3C(C_6H_{10})OH$	145.27	6[3], 126	0.902		43–46		79	i aq
b544	4-*tert*-Butylcyclohexanol	$(CH_3)_3C(C_6H_{10})OH$	156.27	6[1], 18			62–70	115^{15mm}	105	i aq
b545	2-*tert*-Butylcyclohexanone	$(CH_3)_3C(C_6H_9)(=O)$	154.25	7[3], 143	0.896	1.4565^{20}		63^{4mm}	72	
b546	4-*tert*-Butylcyclohexanone	$(CH_3)_3C(C_6H_9)(=O)$	154.25	7[1], 29			47–50	116^{20mm}	96	i aq
b547	Butyl decyl *o*-phthalate	$C_4H_9O_2C_6H_4CO_2C_{10}H_{21}$	362.51		0.994_{25}^{25}				202	
b548	4-*sec*-Butyl-2,6-di-*tert*-butylphenol	$C_2H_5CH(CH_3)C_6H_2(OH)$-$[C(CH_3)_3]$	262.44	6,*3*, 2094	0.902		25	142^{10mm}	>110	

Butyl bromide, b274
sec-Butyl bromide, b275
tert-Butyl bromide, b372
N-Butyl-1-butanamine, d139
Butyl butenoate, b531
Butyl carbitol, b495
Butyl cellosolve, b493
Butyl cellosolve acetate, b497
Butyl chloride, c75
tert-Butyl chloride, c180
2-*tert*-Butyl-*o*-cresol, b574
2-*tert*-Butyl-*p*-cresol, b573
Butyl cyanide, p35



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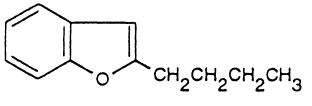


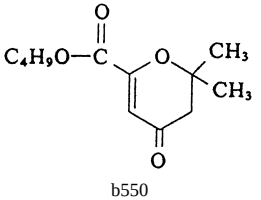
b525

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b549	*N*-Butyldiethanolamine	$C_4H_9N(CH_2CH_2OH)_2$	161.25	4, 285	0.986_{20}^{20}	1.4625^{20}	−70	276	126	
b550	Butyl 3,4-dihydro-2,2-dimethyl-4-oxo-2*H*-pyran-6-carboxylate		226.27		1.054_{25}^{25}	1.4767^{20}		256–270	>110	
b551	*tert*-Butyldimethylchlorosilane	$(CH_3)_3CSi(CH_3)_2Cl$	150.73	4,*4*, 4076			89	124–126	22	
b552	6-*tert*-Butyl-2,4-dimethylphenol	$(CH_3)_3CC_6H_2(CH_3)_2OH$	178.28	6[3], 2020		1.5178^{20}	23	249	111	
b553	*N*-Butylethanolamine	$HOCH_2CH_2NHC_4H_9$	117.19		0.89^{20}	1.444^{20}	−3.5	192	77	
b554	Butyl ethyl ether	$C_4H_9OC_2H_5$	102.18	1, 369	0.7495_4^{20}	1.3818^{20}	−124	92	4	i aq; misc alc, eth
b555	2-Butyl-2-ethyl-1,5-pentanediamine	$H_2N(CH_2)_3C[(CH_2)_3CH_3](C_2H_5)CH_2NH_2$	186.34		0.876	1.4700^{20}		269^{750mm}	>110	
b556	2-Butyl-2-ethyl-1,3-propanediol	$HOCH_2C(C_2H_5)(C_4H_9)CH_2OH$	160.25	1[3], 2228	0.931_{20}^{50}	1.4587^{25}	41–44	178^{50mm}	>110	0.8 aq
b557	Butyl ethyl sulfide	$C_4H_9SC_2H_5$	118.24	1[3], 1522	0.8376_4^{20}	1.4491^{20}	−95.1	144.2		s chl
b558	*N*-*tert*-Butylformamide	$HCONHC(CH_3)_3$	101.15	4[3], 324	0.903	1.4330^{20}	16	202	95	
b559	Butyl formate	$HCO_2C_4H_9$	102.13	2, 21	0.892	1.3889^{20}	−91.5	106	18	
b560	Butyl glycidyl ether	$H_2C(O)CHCH_2OC_4H_9$								
b561	*tert*-Butyl glycidyl ether	$H_2C(O)CHCH_2OC(CH_3)_3$	130.19	17[3], 988	0.917	1.4166^{20}			43	
b562	*tert*-Butylhydrazine HCl	$(CH_3)_3CNHNH_2 \cdot HCl$	124.61	4[3], 1734			194			
b563	*tert*-Butyl hydroperoxide	$(CH_3)_3C{-}O{-}OH$	90.12	1[3], 1579	0.896_4^{20}	1.4007^{20}	−8	34^{17mm}	37	s aq, alc, chl, eth
b564	1-Butylimidazole		124.19	23[2], 36	0.945	1.4800^{20}		116^{12mm}	>110	
b565	Butyl isocyanate	C_4H_9NCO	99.13		0.880	1.4061^{20}		115	17	
b566	*tert*-Butyl isocyanate	$(CH_3)_3CNCO$	99.13	4, 175	0.868	1.3865^{20}		86	−4	
b567	Butyl lactate	$CH_3CH(OH)CO_2C_4H_9$	148.19	3[2], 207	0.984	1.4210^{20}	−28	185–187	69	
b568	Butyl levulinate	$CH_3COCH_2CH_2CO_2C_4H_9$	172.22		0.974	1.4270^{20}		$108^{5.5mm}$	91	

b569	Butyl 3-mercapto-propionate	$HSCH_2CH_2CO_2C_4H_9$	162.25		0.795	1.4100^{20}		101^{12mm}	93	
b570	Butyl methacrylate	$H_2C{=}C(CH_3)CO_2C_4H_9$	142.19	2^3, 1286	0.889^{25}_{15}	1.4230^{25}		170	50	i aq; misc alc, eth
b571	*sec*-Butyl-2-methyl-2-butenoate	$CH_3CH{=}C(CH_3)CO_2$-$CH(CH_3)C_2H_5$	156.23		0.889	1.4350^{20}		85^{27mm}	66	
b572	*tert*-Butyl methyl ether	$(CH_3)_3C{-}O{-}CH_3$	88.15	1, 381	0.7404^{20}_{4}	1.3689^{20}	−109	52	−28	4.8 aq; v s alc, eth; unstable acid solns
b573	2-*tert*-Butyl-4-methyl-phenol	$(CH_3)_3CC_6H_3(CH_3)OH$	164.25		0.9247^{75}_{4}	1.4969^{75}	51.7	237	100	i aq; s org solv
b574	2-*tert*-Butyl-5-methyl-phenol	$(CH_3)_3CC_6H_3(CH_3)OH$	164.25	6^2, 507	0.964	1.5192^{20}		118^{12mm}	105	
b575	2-*tert*-Butyl-6-methyl-phenol	$(CH_3)_3CC_6H_3(CH_3)OH$	164.25			1.5190^{20}	30–32	230	107	
b576	*tert*-Butyl-1-methyl-2-propynyl ether	$(CH_3)_3COCH(CH_3)C{\equiv}CH$	126.20		0.795	1.4100^{20}		41^{25mm}	10	
b577	*tert*-Butyl methyl sulfide	$(CH_3)_3CSCH_3$	104.21	1^3, 1591	0.826^{20}_{4}	1.441^{20}	−97.8	102	−3	v s alc
b578	Butyl nitrite	C_4H_9ONO	103.12	1, 369	0.9114^{0}_{4}	1.3768		78	−13	misc alc, eth
b579	*tert*-Butyl nitrite	$(CH_3)_3CONO$	103.12	1, 382	0.8671^{20}_{4}	1.3687^{20}		63	−13	sl s aq; v s alc, chl, eth, CS_2

Butyl diglyme, b151
tert-Butyldihydroxybenzene, b534
Butyl disulfide, d146
tert-Butyl disulfide, d147
1-Butylene, b477
cis-2-Butylene, b478
trans-2-Butylene, b479
1,4-Butylene bis(2,3-epoxypropyl) ether, b185
1,3-Butylene glycol, b456
1,4-Butylene glycol, b457
2,3-Butylene glycol, b458
1,3-Butyleneglycol methyl ether, m64
1,2-Butylene oxide, e3
Butyl ether, d148
Butyl ethyl ketone, h15
tert-Butyl fluoride, f22
Butyl glycol, b493
2,2′-(Butylimino)diethanol, b549
Butyl iodides, i26, i27, i38
Butyl levulinate, b582
Butyl mercaptans, b470, b471; m394, m395, m396
Butyl methanoate, b559
Butyl methyl ketone, d572



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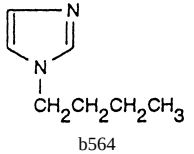


b564

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

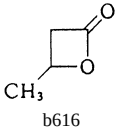
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b580	Butyl 4-nitrobenzoate	$O_2NC_6H_4CO_2C_4H_9$	223.23	9^2, 259			35–39	160^{8mm}	>110	
b581	Butyl octadecanoate	$CH_3(CH_2)_{16}CO_2C_4H_9$	340.60	2^2, 352	0.8551_4^{20}	1.4422^{25}	26.3	343	160	s alc; v s acet
b581a	Butyl *cis*-9-octadecenoate	$CH_3(CH_2)_8CH{=}CH(CH_2)_7CO_2C_4H_7$	338.57		0.8704^{15}	1.4480^{25}	−26		180	s eth
b582	Butyl 4-oxopentanoate	$CH_3C(=O)CH_2CH_2CO_2C_4H_9$	172.22		0.9735_4^{20}	1.4270^{20}		107^{6mm}	91	s alc, acet, eth
b583	4-(1-Butylpentyl)-pyridine	$C_4H_9CHC(CH_2)_3CH_3$ | C_5H_4N	205.35	20^3, 2872	0.887	1.4877^{20}		267	>110	
b584	*tert*-Butyl peroxobenzoate	$C_6H_5C(=O)O{-}O{-}C(CH_3)_3$	194.23		1.021	1.4990^{20}		$76^{0.2mm}$	93	
b585	2-*sec*-Butylphenol	$CH_3CH_2CH(CH_3)C_6H_4OH$	150.22		0.982	1.5222^{20}	12	228	112	i aq; s alc; v s eth
b586	2-*tert*-Butylphenol	$(CH_3)_3CC_6H_4OH$	150.22	6^2, 489	0.9783_4^{20}	1.5228^{20}	−7	221–224	>110	
b587	4-*sec*-Butylphenol	$CH_3CH_2CH(CH_3)C_6H_4OH$	150.22	6, 522	0.969_4^{20}	1.5150	62	136^{25mm}	115	s hot aq, alc, eth
b588	4-*tert*-Butylphenol	$(CH_3)_3CC_6H_4OH$	150.22	6, 524	0.908_4^{114}	1.4787^{114}	98	237		i aq; s alc, eth
b589	*tert*-Butyl 4-phenoxyphenol ketone	$C_6H_5OC_6H_4C(=O)C(CH_3)_3$	254.33	8^3, 491			52–54	175^{3mm}	>110	
b590	*tert*-Butyl phenyl carbonate	$C_6H_5OC(=O)OC(CH_3)_3$	194.23		1.047	1.4805^{20}		$79^{0.8mm}$	101	
b591	Butyl phenyl ether	$CH_3CH_2CH_2CH_2OC_6H_5$	150.22	6, 143	0.9351_4^{20}	1.4970^{20}	−19	210.3	82 (OC)	
b592	4-*tert*-Butylphenyl salicylate	$HOC_6H_4CO_2CH_6H_4C(CH_3)_3$	270.31				62–64			<0.1 aq; 79 alc; 153 EtOAc; 158 toluene
b593	Butyl propionate	$CH_3CH_2CO_2C_4H_9$	130.19	2, 241	0.8818^{15}	1.3982^{25}	−89	146.8	38	v s alc, eth; v sl s aq
b594	*tert*-Butyl propionate	$CH_3CH_2CO_2C(CH_3)_3$	130.19	2^3, 528	0.865	1.3930^{20}		118	20	
b595	4-*tert*-Butyl pyridine	$(CH_3)_3C(C_5H_4N)$	135.21	20, 252	0.915	1.4952^{20}		197	63	
b596	*tert*-Butyl 1-pyrrolecarboxylate	$(C_4H_4N)CO_2C(CH_3)_3$	167.21		1.000	1.4685^{20}		92^{20mm}	75	
b597	1-Butylpyrrolidine	$(C_4H_8N)C_4H_9$	127.23	20^2, 4	0.814	1.4440^{20}		157	36	
b598	4-*tert*-Butylstyrene	$(CH_3)_3CC_6H_4CH{=}CH_2$	160.26	5^3, 1254	0.875	1.5260^{20}	−37	92^{9mm}	80	
b599	1-Butyl-3-sulfanilylurea	$4\text{-}(H_2N)C_6H_4SO_2NHCONHC_4H_9$	271.34	14,*4*, 2667			143–145			
b600	Butyltin trichloride	$C_4H_9SnCl_3$	282.17	4^4, 4346	1.693	1.5229^{20}		93^{10mm}	81	
b601	Butyltin tris(2-ethylhexanoate)	$[CH_3(CH_2)_3CH(C_2H_5)CO_2]_3SnC_4H_9$	605.43		1.105	1.4650^{20}			>110	

b602	4-*tert*-Butyltoluene	$(CH_3)_3CC_6H_4CH_3$	148.25	5, 439	0.8612^{20}	1.4918^{20}	−52	190	68	
b603	Butyltrichlorosilane	$C_4H_9SiCl_3$	191.56	4,*1*, 582	1.160	1.4370^{20}		149	45	
b604	*tert*-Butyltrichlorosilane	$(CH_3)_3CSiCl_3$	191.56	4^3, 1905			97–100	132–134	40	
b605	Butyl trifluoroacetate	$CF_3CO_2C_4H_9$	170.1		1.0268^{22}	1.353^{22}		100.1		
b606	Butyltrimethoxysilane	$C_4H_9Si(OCH_3)_3$	178.3		0.9312_4^{20}	1.3979^{20}		164–165		
b607	*tert*-Butyl trimethylsilyl peroxide	$(CH_3)_3C{-}O{-}O{-}Si(CH_3)_3$	162.3		0.8219_4^{20}	1.3935^{20}	dec 135	41^{41mm}		
b608	Butylurea	$C_4H_9NHCONH_2$	116.16	4^1, 371			96–98			s aq, alc, eth
b609	Butyl vinyl ether	$C_4H_9OCH{=}CH_2$	100.16		0.7792^{20}	1.4007^{20}	−92	94.2	−9	0.3 aq
b610	5-*tert*-Butyl-*m*-xylene	$(CH_3)_3CC_6H_3(CH_3)_2$	162.28	5, 447	0.867	1.4946^{20}		205–206	72	
b610a	1-Butyne	$CH_3CH_2C{\equiv}CH$	54.09		2.211 g/L		−126	8.1		
b610b	2-Butyne	$CH_3C{\equiv}C{-}CH_3$	54.09		0.688		−32	27		
b611	2-Butyne-1,4-diol	$HOCH_2C{\equiv}CCH_2OH$	86.09	1^1, 261		1.450^{25}	56–58	238	152	374 aq; 83 als; 0.04 bz; 2.6 eth; 70 acet
b612	Butyraldehyde	$CH_3CH_2CH_2CHO$	72.11	1, 662	0.8016_4^{20}	1.3843^{20}	−96/−99	74.8	−22	7.1 aq; misc alc, acet, eth, EtOAc
b613	Butyramide	$CH_3CH_2CH_2CONH_2$	87.12	2, 275			116	216		16 aq; s alc
b614	Butyric acid	$CH_3CH_2CH_2COOH$	88.11	2, 264	0.9582_4^{20}	1.3991^{20}	−5.3/−5.7	163.5	72	misc aq, alc, eth
b615	Butyric anhydride	$[CH_3CH_2CH_2C(=O)]_2O$	158.20	2, 274	0.9668_4^{20}	1.4070^{20}	−75/−66	199.5	54	s aq (dec); alc (dec), eth
b616	β-Butyrolactone		86.09	17^1, 130	1.056	1.4109^{20}	−43.5	204	60	
b617	γ-Butyrolactone		86.09	17, 234	1.124_4^{25}	1.4348^{25}	−43.5	204	98	misc aq; s alc, acet, bz, eth
b618	Butyronitrile	$CH_3CH_2CH_2CN$	69.11	2^2, 252	0.7954_4^{15}	1.4440^{20}	−112	117.6	24	3.3 aq; misc alc, eth

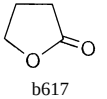
Butyl oleate, b581a
tert-Butyl perbenzoate, b584
Butyl *o*-phthalate, d165
Butyl 2-propenoate, b507a

Butyl propyl ketone, o38
Butyl stearate, b581
Butyl sulfate, d169
Butyl sulfide, d170

tert-Butyl sulfide, d171
Butyl sulfite, d172
Butyl sulfone, d173
γ-Butyrolactam, p285



b616



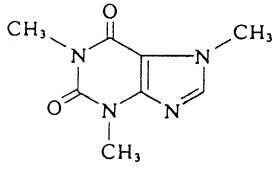
b617

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

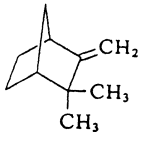
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
b619	Butyrophenone	$C_6H_5C(=O)C_3H_7$	148.21	7, 313	1.021	1.5195^{20}	11–13	230	88	
b620	Butyryl chloride	$CH_3CH_2CH_2COCl$	106.55	2, 274	1.0263_4^{21}	1.412^{20}	−89	102	21	s aq (dec), alc (dec); misc eth
c1	Caffeine		194.19	26, 461	1.23_4^{18}		238	subl 178		2.1 aq; 1.5 alc; 18 chl; 0.19 eth; 1 bz; 2 acet
c2	(±)-Camphene		136.24	5, 156	0.8422_4^{54}	1.4551^{54}	51–52	159	36	i aq; s alc, chl, eth
c3	(1*R*)-(+)-Camphor		152.24	7, 101	0.992_4^{25}	1.5462	179	207	66	100 alc; 100 eth; 200 chl; 250 acet
c4	(1*R*,3*S*)-Camphoric acid		200.23	9, 745	1.186_4^{20}		186–188			at 25°C: 0.8 aq, 100 alc, 250 acet, 200 eth, 200 HOAc; s chl
c5	(±)-10-Camphor-sulfonic acid		232.30	11, 314			194 dec			deliq moist air; sl s HOAc, EtOAc; i eth
c6	Carbazole		167.21	20, 433	1.10_4^{18}		245	355		16 pyr; 11 acet; 3 eth; 0.8 bz; sl s HOAc, PE
c7	4-Carbethoxy-2-methyl-3-cyclo-hexen-1-one		182.22	10, 631	1.078	1.4880^{20}		268–272	>110	
c8	Carbobenzyloxy-glycine	$C_6H_5CH_2OC(=O)NH-CH_2COOH$	209.20				122			
c9	Carbohydrazide	$H_2NNHC(=O)NHNH_2$	90.08	3, 121			157–158			v s aq; i alc, bz, eth; forms salts with acids
c10	Carbon disulfide	CS_2	76.14	3, 197	1.2632_4^{20}	1.6270^{20}	−111.6	46.5	−30	0.3 aq; misc bz, chl, eth, CCl_4
c11	Carbon monoxide	CO	28.01	Merck: 12, 1861	1.145 g/L		−205	−191.5		2.3 aq; 16 alc; s chl, EtOAc, HOAc
c12	Carbon oxide sulfide	COS	60.07		2.456 g/L		−138.8	−50		
c13	Carbon tetrabromide	CBr_4	331.65	1, 68	3.42		90	190	none	

c14	Carbon tetrachloride	CCl_4	153.82	1, 64	1.589_{25}^{25}	1.4607^{20}	−23	76.7	none	0.05 aq; misc alc, bz, chl, eth, CS_2, PE
c15	Carbon tetrafluoride	CF_4	88.01	1, 59	1.89^{-183} liq		−183.6	−127.8		
c16	Carbon tetraiodide	CI_4	519.63	1, 74	4.32_4^{20}		171			s bz, chl; dec hot alc
c17	4-Carboxybenzene-sulfonamide	$HOOCC_6H_4SO_2NH_2$	201.20	11, 390			dec 280			v s alc; s alkalis; i aq, bz, eth

Cadaverine, p30
2-Camphanone, c3
Capraldehyde, d7
Capric acid, d15
Capric alcohol, d16
Caproaldehyde, h51
Caproic acid, h64
Caproic anhydride, h65
6-(or ϵ)-Caprolactam, o61
ϵ-Caprolactone, h69
Capronitrile, h61
Caproyl chloride, h72
Capryl alcohol, o32
Caprylaldehyde, o43
Caprylic acid, o30
Caprylonitrile, o28
Capryloyl chloride, o39
N-(Carbamoylmethyl)iminodiacetic acid, a14
Carbamylurea, b238
Carbanilide, d775
Carbazole, d751
Carbitol, e41a
Carbitol acetate, e42
Carbobenzoxy chloride, b91
Carbolic acid, p65
3-Carbomethoxypropionyl chloride, m195
Carbon bromotrichloride, b432
N-Carbonylsulfamyl chloride, c249
Carbonyl sulfide, c12
Carboxybenzaldehyde, f37



c1



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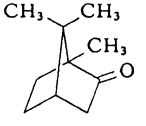

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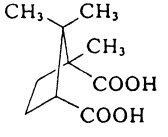

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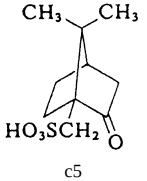

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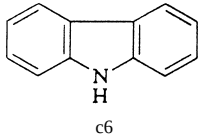
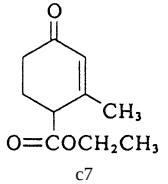


c6



c7

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
c18	(4-Carboxybutyl)triphenylphosphonium bromide	$HOOC(CH_2)_4(C_6H_5)_3Br$	443.33				205–207			
c19	1-(Carboxymethyl)-pyridinium chloride		173.60				189 dec			
c20	*R*-(−)-Carvone		150.22	7, 157	0.965_4^{20}	1.4989^{20}	<15	230	88	i aq; misc alc
c21	Catechol	C_6H_4-1,2-$(OH)_2$	110.11		1.344		104–106	245	137	43 aq; v s alkalis, pyr; s alc, bz, chl, eth
c22	Catecholborane		119.92		1.125	1.5070^{20}	12	50^{50mm}	2	
c23	Chalcone	$C_6H_5CH{=}CHCOC_6H_5$	208.26	7, 478	1.0712_4^{62}		55–57	208^{25mm}	>110	v s bz, chl, CS_2, eth; sl s alc
c23a	Chloroacetaldehyde	$ClCH_2CHO$	78.50	1, 610			−16	85–86		s aq, alc, eth
c24	2-Chloroacetamide	$ClCH_2CONH_2$	93.51	2, 199			119	225 dec		10 aq; 10 alc; sl s eth
c25	2′-Chloroacetanilide	$ClC_6H_4NHCOCH_3$	169.61	12, 559			88–90			s alc
c26	3′-Chloroacetanilide	$ClC_6H_4NHCOCH_3$	169.61	12, 604			79–81			v s alc, bz, CS_2
c26a	4′-Chloroacetanilide	$ClC_6H_4NHCOCH_3$	169.61	12, 611	1.385_4^{20}		179			i aq; v s alc, eth, CS_2
c27	Chloroacetic acid	$ClCH_2COOH$	94.50	2, 194	1.580 (*c*)	1.4297^{65}	61	189	126	v s aq; s alc, bz, eth
c28	Chloroacetic anhydride	$[ClCH_2C(=O)]_2O$	170.98	2, 199	1.5494_4^{20}		46	203		v s chl, eth; sl s bz; dec by aq, alc
c29	4′-Chloroacetoacetanilide	$CH_3COCH_2CH_2CONHC_6H_4Cl$	211.65				134	dec	160 (CC)	
c30	Chloroacetonitrile	$ClCH_2CN$	75.50	2, 201	1.193	1.4225^{20}		126	47	
c31	2-Chloroacetophenone	$C_6H_5COCH_2Cl$	154.60	7, 282	1.324^{15}		54–56	245		i aq; v s alc, bz, eth
c32	*o*-Chloroacetophenone	$ClC_6H_4COCH_3$	154.60	7^1, 151	1.188	1.5438^{20}		228^{738mm}	88	sl s aq; s eth
c33	*p*-Chloroacetophenone	$ClC_6H_4COCH_3$	154.60	7, 281	1.192_4^{20}	1.555^{20}	20–21	237	90	i aq; misc alc, eth
c34	Chloroacetyl chloride	$ClCH_2COCl$	112.94	2, 199	1.420_4^{20}	1.4541^{20}	−21.8	106	none	dec by aq, MeOH
c36	2-Chloroacrylonitrile	$H_2C{=}C(Cl)CN$	87.51		1.096	1.4290^{20}	−65	89	6	
c37	2-Chloro-4-aminotoluene	$ClC_6H_3(CH_3)NH_2$	141.60	12, 988	1.1671	1.5840^{20}	24–25	238	100	
c38	2-Chloroaniline	$ClC_6H_4NH_2$	127.57	12, 597	1.2125_4^{20}	1.5895^{20}	−14	208.8	97	0.88 aq; s acids, most common org solvents
c39	3-Chloroaniline	$ClC_6H_4NH_2$	127.57	12, 602	1.2150_4^{22}	1.5931^{20}	−10.4	230.5	123	i aq; s most common org solvents

c40	4-Chloroaniline	$ClC_6H_4NH_2$	127.57	12, 607	1.169_4^{77}	1.5546^{85}	72.5	232		s hot aq; v s alc, acet, eth, CS_2
c41	1-Chloroanthra-quinone		242.66	7, 787			160	sublimes		sl s alc; s hot bz; misc eth
c42	2-Chloroanthra-quinone		242.66	7, 787			211	sublimes		sl s alc, bz; i eth
c43	2-Chlorobenzaldehyde	ClC_6H_4CHO	140.57	7, 233	1.2483_4^{20}	1.5658	11	215	87	sl s aq; s alc, bz, eth
c44	3-Chlorobenzaldehyde	ClC_6H_4CHO	140.57	7, 234	1.241	1.5545^{20}	18	214	88	
c45	4-Chlorobenzaldehyde	ClC_6H_4CHO	140.57	7, 235	1.196_4^{61}	1.552^{61}	47	214	87	s aq; v s alc, bz, eth
c46	2-Chlorobenzamide	$ClC_6H_4CONH_2$	155.58	9, 336			142–144			
c47	Chlorobenzene	C_6H_5Cl	112.56	5, 199	1.1063^{20}	1.5248^{20}	−45.3	131.7	28	0.049 aq[30]; v s alc, bz, chl, eth
c48	4-Chlorobenzene-sulfonamide	$ClC_6H_4SO_2NH_2$	191.64	11, 55			146			s hot aq, hot alc, hot eth
c49	4-Chlorobenzene-sulfonic acid	$ClC_6H_4SO_3H$	192.62	11, 54				149^{22mm}	107	
c50	4-Chlorobenzene-sulfonyl chloride	$ClC_6H_4SO_2Cl$	211.07	11, 55			55	141^{15mm}	107	dec aq, alc; v s bz, eth
c51	2-Chlorobenzoic acid	ClC_6H_4COOH	156.57	9, 334	1.544_4^{20}		140			0.11 aq; v s alc, eth

(3-Carboxy-2-hydroxypropyl)trimentylammonium hydroxide, c19
(Carboxylmethyl)trimethylammonium hydroxide, b133
(Carbomethylimino)bis(ethylenenitrilo)-tetraacetic acid, d363
3-Carboxylpropyl disulfide, d809
Carvene, L17
Cellosolve, e40
Cellosolve acetate, e42
Cetyl alcohol, h35
Cetyl bromide, b345
Chalcone, d768
Chloral, t218
Chloramine T, c258
Chloranil, t34, t35
Chlorendic anhydride, h28
Chloroacetaldehyde diethyl acetal, c96
Chloroacetaldehyde dimethyl acetal, c105
Chloroacetone, c229a
Chloroenthranilic acid, a138
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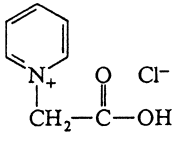
Chlorobenzeneamines, c38 thru c40
p-Chlorobenzenethiol, c252



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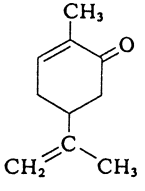

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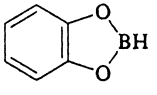

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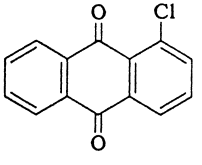

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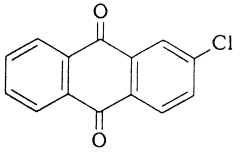


c42

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
c52	3-Chlorobenzoic acid	ClC_6H_4COOH	156.57	9, 337	1.496_4^{25}		158			0.04 aq; v s alc, eth
c53	4-Chlorobenzoic acid	ClC_6H_4COOH	156.57	9, 340			241–243			0.02 aq; v s alc, eth
c54	2-Chlorobenzonitrile	ClC_6H_4CN	137.57	9, 336			46	232	108	s alc, eth
c55	4-Chlorobenzonitrile	ClC_6H_4CN	137.57	9, 341			93	223		s alc, bz, chl, eth
c56	2-Chlorobenzophenone	$ClC_6H_4COC_6H_5$	216.67	7, 419			44–47	300	>110	
c57	4-Chlorobenzophenone	$ClC_6H_4COC_6H_5$	216.67	7, 419			77	196^{17mm}		s alc, acet, bz, eth
c58	2-Chlorobenzotrichloride	$ClC_6H_4CCl_3$	229.92	5, 302	1.508	1.5817^{20}	29	264	98	
c59	4-Chlorobenzotrichloride	$ClC_6H_4CCl_3$	229.92	5, 303	1.495	1.5722^{20}		245	>110	
c60	2-Chlorobenzotrifluoride	$ClC_6H_4CF_3$	180.56	5^3, 692	1.3540^{25}	1.4513^{25}	−6.4	152	58	
c61	3-Chlorobenzotrifluoride	$ClC_6H_4CF_3$	180.56	5^3, 692	1.3311^{25}	1.4438^{25}	−56.7	137.7	38	
c62	4-Chlorobenzotrifluoride	$ClC_6H_4CF_3$	180.56		1.353^{20}	1.4463	−36	138.7	47	
c63	2-(4-Chlorobenzoyl)-benzoic acid	$ClC_6H_4COC_6H_4COOH$	260.68	10, 750			150			s alc, bz, eth
c64	2-Chlorobenzoyl chloride	ClC_6H_4COCl	175.01	9, 336	1.382	1.5718^{20}	−3	238	>110	dec by aq & alc
c65	4-Chlorobenzoyl chloride	ClC_6H_4COCl	175.01	9, 341	1.377	1.5780^{20}	14	222	105	dec by aq & alc
c66	4-Chlorobenzyl alcohol	$ClC_6H_4CH_2OH$	142.59	6, 444			72	234		v s alc, eth
c67	2-Chlorobenzylamine	$ClC_6H_4CH_2NH_2$	141.60	12, 1073	1.173	1.5630^{20}		104^{11mm}	88	
c68	4-Chlorobenzylamine	$ClC_6H_4CH_2NH_2$	141.60	12, 1074	1.164	1.5586^{20}		215	90	
c69	2-Chlorobenzyl chloride	$ClC_6H_4CH_2Cl$	161.03	5, 297	1.274	1.5591^{20}	−17	214	82	
c70	4-Chlorobenzyl chloride	$ClC_6H_4CH_2Cl$	161.03	5, 308			30	222	97	s alc, v s eth
c71	2-Chlorobenzyl cyanide	$ClC_6H_4CH_2CN$	151.60	9, 448		1.5540^{20}	24	242	>110	

c72	4-Chlorobenzyl cyanide	$ClC_6H_4CH_2CN$	151.60	9, 448			30.3	267	>110	
c73	4-Chlorobenzyl mercaptan	$ClC_6H_4CH_2SH$	158.65	6, 466	1.202	1.5893^{20}	20		76	
c74	1-Chloro-1,3-butadiene	$H_2C{=}CHCH{=}CHCl$	88.54	1^3, 949	0.9601^{20}_4	1.4712^{20}		68	−20	v s chl
c74a	2-Chloro-1,3-butadiene	$H_2C{=}CHC(Cl){=}CH_2$	88.54		0.952			59		
c75	1-Chlorobutane	$CH_3CH_2CH_2CH_2Cl$	92.57	1, 118	0.8864^{20}_4	1.4021^{20}	−123.1	78.4	−9	0.11 aq; misc alc, eth
c76	2-Chlorobutane	$CH_3CH_2CH(Cl)CH_3$	92.57	1, 119	0.8732^{20}_4	1.3971^{20}	−131.3	68.2	−15	0.1 aq; misc alc, eth
c77	4-Chloro-1-butanol	$ClCH_2CH_2CH_2CH_2OH$	108.56	1^2, 398	1.0883^{20}_4	1.4518^{20}		89^{20mm}	32	s alc, eth
c78	3-Chloro-2-butanone	$CH_3CH(Cl)C(=O)CH_3$	106.55	1, 669	1.055	1.4172^{20}		117	21	v s alc, eth
c79	*cis*-1-Chloro-2-butene	$CH_3CH{=}CHCH_2Cl$	90.55	1^2, 176	0.9426^{20}	1.4390^{20}		84.1	−15	s alc, acet
c80	*trans*-1-Chloro-2-butene	$CH_3CH{=}CHCH_2Cl$	90.55	1^2, 176	0.929	1.4390^{20}		85	−5	s alc, acet
c81	3-Chloro-1-butene	$CH_3CH(Cl)CH{=}CH_2$	90.55	1^2, 174	0.9001^{20}_4	1.4155^{20}		65	−20	v s acet
c82	4-Chlorobutyl acetate	$CH_3CO_2CH_2CH_2CH_2CH_2Cl$	150.61	2^2, 141	1.072	1.4338^{20}		92^{22mm}	64	
c83	3-Chloro-1-butyne	$CH_3CH(Cl)C{\equiv}CH$	88.54	1^4, 970	0.961	1.4280^{20}		68–70	1	
c84	3-Chlorobutyric acid	$CH_3CH(Cl)CH_2COOH$	122.55	2, 277	1.186^{20}_4	1.4421^{20}	16.3	109^{17mm}	>110	s alc, eth
c85	4-Chlorobutyric acid	$ClCH_2CH_2CH_2COOH$	122.55	2, 278	1.2236^{20}_4	1.4521^{20}	12–16	196^{22mm}	>110	sl s aq; v s eth
c86	4-Chlorobutyronitrile	$ClCH_2CH_2CH_2CN$	103.55	2, 278	1.158	1.4413^{20}		197	85	s alc, eth
c87	4-Chlorobutyryl chloride	$ClCH_2CH_2CH_2COCl$	141.00	2, 278	1.258	1.4609^{20}		174	72	dec by aq, alc; s eth
c88	Chloro(chloromethyl)-dimethylsilane	$ClCH_2Si(CH_3)_2Cl$	143.09		1.086	1.4373^{20}		114^{752mm}	21	
c89	3-Chloro-2-chloromethyl-1-propene	$H_2C{=}C(CH_2Cl)_2$	125.00	1^2, 181	1.080	1.4753^{20}	−14	138	36	
c90	*trans*-2-Chlorocinnamic acid	$ClC_6H_4CH{=}CHCO_2H$	182.61	9, 594			208–210			
c91	Chlorocyclohexane	ClC_6H_{11}	118.61	5, 21	1.000^{20}_4	1.4620^{20}	−44	142	28	i aq; s alc, eth
c92	1-Chloro-3-cyclohexylpropane	$C_6H_{11}(CH_2)_3Cl$	160.69	5^2, 23	0.997	1.4662^{20}		79^{5mm}	78	
c93	Chlorocyclopentane	C_5H_9Cl	104.58	5, 19	1.0051^{20}_4	1.4512^{20}		114	15	i aq
c94	1-Chlorodecane	$CH_3(CH_2)_9Cl$	176.73	1, 168	0.868	1.4362^{20}	−34	223	83	i aq
c95	Chlorodicyclohexylborane	$(C_6H_{11})_2BCl$	212.57	16^4, 1637	0.970			101^{1mm}		
c96	2-Chloro-1,1-diethoxyethane	$ClCH_2CH(OC_2H_5)_2$	152.62	1, 611	1.018	1.4157^{20}		157	29	

Chlorocresol, c176, c177 Chlorodibromomethane, d88 2-Chloro-*N*,*N*-diethylethylamine, d328

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
c97	3-Chloro-1,1-diethoxy-propane	$ClCH_2CH_2CH(OC_2H_5)_2$	166.65	1, 632	0.995	1.4240^{20}		84^{25mm}	36	
c98	Chlorodifluoroacetic acid	$F_2C(Cl)COOH$	130.48	2, 201	1.540	1.3559^{20}	24–26	122	none	
c99	1-Chloro-2,4-difluoro-benzene	$ClC_6H_3F_2$	148.54	5^4, 653	1.353	1.4750^{20}		127	32	
c100	1-Chloro-1,1-difluoro-ethane	$CH_3C(Cl)F_2$	100.50	1^3, 138	4.108 g/L		−131	−10		0.19 aq
c100a	1-Chloro-2,2-difluoro-ethylene	$ClCH{=}CF_2$	98.48		4.025 g/L		−138.5	−18.5		
c101	Chlorodifluoro-methane	$HCClF_2$	86.47	1^3, 41	1.4909^{-69}		−157	−40.8		0.30 aq
c102	1-Chloro-2,4-di-hydroxybenzene	$ClC_6H_3(OH)_2$	144.56	6^2, 818			107	147^{18mm}		v s aq, alc, chl, eth
c103	2-Chloro-1,4-di-hydroxybenzene	$ClC_6H_3(OH)_2$	144.56	6, 849			101–102	263		v s aq; i alc, s eth
c104	2-Chloro-1,4-di-methoxybenzene	$ClC_6H_3(OCH_3)_2$	172.61	6^3, 4432	1.211	1.5467^{20}		234	110	
c105	2-Chloro-1,1-di-methoxyethane	$ClCH_2CH(OCH_3)_2$	124.57		1.094^{20}_{20}	1.4148^{20}		130	28	
c107	2-Chloro-4,6-di-methylaniline	$ClC_6H_2(CH_3)_2NH_2$	155.63	12, 1125	1.110		38–40		>110	
c108	4-Chloro-3,5-di-methylphenol	$ClC_6H_2(CH_3)_2OH$	156.61	6^2, 463			115.5	246		0.03 aq; 100 alc; s bz, eth, alkalis
c109	1-Chloro-2,2-di-methylpropane	$(CH_3)_3CCH_2Cl$	106.59	1, 141	0.866^{20}_4	1.4042^{20}	−20	84.4	32	
c110	3-Chloro-2,2-dimethyl-1-propanol	$ClCH_2C(CH_3)_2CH_2OH$	122.60			1.4504^{20}	34–36	87^{35mm}	71	
c111	Chlorodimethylsilane	$(CH_3)_2Si(Cl)H$	94.62		0.852^{20}_4	1.3827^{20}	−111	36	−28	
c112	Chlorodimethylvinyl-silane	$(CH_3)_2Si(Cl)CH{=}CH_2$	120.7	*4,4*, 4080	0.884^{25}_4	1.414^{25}		82.5	−5	
c113	6-Chloro-2,4-dinitro-aniline	$ClC_6H_2(NO_2)_2NH_2$	217.57	12^1, 367			159			

c114	1-Chloro-2,4-dinitrobenzene	$ClC_6H_3(NO_2)_2$	202.55	5, 263	1.4982_4^{75}	1.5857^{60}	52–54	315	186	sl s alc; s hot alc, bz, eth
c115	2-Chloro-3,5-dinitrobenzoic acid	$ClC_6H_2(NO_2)_2COOH$	246.56	9, 415			198	241 explodes		0.3 aq
c116	Chlorodiphenylmethane	$C_6H_5CH(Cl)C_6H_5$	202.68	5^2, 500	1.140_4^{20}	1.5951^{20}	17	140^{3mm}	>110	
c117	Chlorodiphenylmethylsilane	$(C_6H_5)_2Si(Cl)CH_3$	232.8	16^2, 606	1.1277_4^{20}	1.5742^{20}		295	>110	
c118	Chlorodiphenylphosphine	$(C_6H_5)_2PCl$	220.64	16, 763	1.229	1.6338^{20}		320	>110	
c119	1-Chlorododecane	$CH_3(CH_2)_{11}Cl$	204.79		0.8673_4^{20}	1.4426	−9	116	93	v s alc; s bz
c120	1-Chloro-2,3-epoxypropane		92.53	17, 6	1.1812_4^{20}	1.4358^{20}	−57.2	116.1	31	5.9 aq; misc alc, chl
c121	Chloroethane	CH_3CH_2Cl	64.52	1, 82	0.9214_4^{0}	1.3742^{10}	−139	12.3	−50	0.45 aq[0]; 48 alc; misc eth
c122	2-Chloroethanol	$ClCH_2CH_2OH$	80.52	1, 337	1.2019^{20}	1.4422^{20}	−67.5	128.6	60	misc aq, alc
c123	2-(2-Chloroethoxy)ethanol	$ClCH_2CH_2OCH_2CH_2OH$	124.57	1, 467	1.180	1.4529^{20}		81^{5mm}	90	
c124	2-[2-(2-Chloroethoxy)ethoxy]ethanol	$ClCH_2CH_2OCH_2CH_2O$-CH_2CH_2OH	168.62	1, 468	1.160	1.4580^{20}		120^{5mm}	107	
c125	2-Chloroethoxytrimethylsilane	$ClCH_2CH_2OSi(CH_3)_3$	152.70	4^3, 1856	0.944	1.4140^{20}		134	30	
c126	2-Chloroethylamine hydrochloride	$ClCH_2CH_2NH_2 \cdot HCl$	115.99	4, 133			146			
c127	1-Chloro-2-ethylbenzene	$ClC_6H_4C_2H_5$	140.61		1.055_{25}^{25}		−81	179.2	66	i aq; misc alc, eth
c128	(2-Chloroethyl)benzene	$C_6H_5CH_2CH_2Cl$	140.61	5, 354	1.069	1.5300^{20}		84^{16mm}	66	s alc, bz, eth
c129	Chloroethylene	$H_2C{=}CHCl$	62.50	1, 186	0.97^{-14}		−154	−13.4	−78	sl s aq; s alc
c130	*N*-(2-Chloroethyl)-*N*-ethylamine	$C_6H_5N(C_2H_5)CH_2CH_2Cl$	183.68	12^3, 263	1.075	1.5584^{20}		164^{42mm}	>110	
c131	2-Chloroethyl ethyl ether	$ClCH_2CH_2OCH_2CH_3$	108.57	1, 337	0.989	1.4120^{20}		107	15	

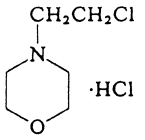
Chlorodimethyl ether, c173 2-Chloroethyl alcohol, c122 2-Chloroethyl ether, b163

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
c132	2-Chloroethyl methyl ether	$ClCH_2CH_2OCH_3$	94.54	1, 337	1.035	1.4090^{20}		90	15	
c133	*N*-(2-Chloroethyl)-morpholine HCl		186.08				186			
c133a	2-Chloroethyl phenyl ether	$C_6H_5OCH_2CH_2Cl$	156.61	6^3, 675	1.129	1.5340^{20}		98^{15mm}	100	
c134	*N*-(2-Chloroethyl)-piperidine HCl		184.11	20, 17			236			
c135	2-Chloroethyl *p*-toluenesulfonate	$CH_3C_6H_4SO_3CH_2CH_2Cl$	234.70	11^2, 45	1.294	1.5290^{20}		$153^{0.3mm}$	>110	
c136	2-Chloroethyl vinyl ether	$H_2C{=}CHOCH_2CH_2Cl$	106.55	1^2, 473	1.0525^{15}_{15}	1.4370^{20}	−69.7	110	16	0.6 aq
c137	1-Chloro-2-fluoro-benzene	ClC_6H_4F	130.55	5^1, 110	1.244	1.5010^{20}	−42.4	138.5	31	s alc, eth
c138	1-Chloro-3-fluoro-benzene	ClC_6H_4F	130.55		1.219	1.4944^{20}		126	20	s alc, eth
c139	2-Chloro-6-fluoro-benzyl chloride	$Cl(F)C_6H_3CH_2Cl$	179.02		1.401	1.5372^{20}			93	
c140	4-Chloro-4′-fluoro-butyrophenone	$FC_6H_4C(=O)CH_2CH_2CH_2Cl$	200.64		1.220	1.5255^{20}			>110	
c141	3-Chloro-4-fluoro-nitrobenzene	$Cl(F)C_6H_3NO_2$	175.55	5^1, 130	1.6028^{17}	1.5674^{17}	41.5	127^{17mm}		
c142	2-Chloro-4-fluoro-phenol	$Cl(F)C_6H_3OH$	146.55	6^4, 880	1.344	1.5300	23	88^{4mm}	75	
c143	2-Chloro-6-fluoro-toluene	$Cl(F)C_6H_3CH_3$	144.58		1.191	1.5026^{20}		156	46	
c144	4-Chloro-2-fluoro-toluene	$Cl(F)C_6H_3CH_3$	144.58	5^4, 813	1.186	1.4998^{20}		158^{743mm}	51	
c145	Chloroform	$CHCl_3$	119.39	1, 61	1.4832^{20}	1.4459^{20}	−63.6	61.1		0.50 aq[25]; misc alc, bz, eth, PE, CCl_4
c146	Chloroform-*d*	$CDCl_3$	120.39	1^3, 63	1.500	1.4445^{20}	−64	60.9		see under chloroform
c147	1-Chloroheptane	$CH_3(CH_2)_6Cl$	134.65	1, 154	0.881^{16}_{0}	1.4250^{20}	−69	159–161	41	misc alc, eth
c148	1-Chlorohexadecane	$CH_3(CH_2)_{15}Cl$	260.89	1, 172	0.865	1.4490^{20}		149^{1mm}	>110	

c149	1-Chlorohexane	$CH_3(CH_2)_5Cl$	120.62	1, 143	0.8780_4^{20}	1.4195^{20}	−94	134	26	i aq
c150	6-Chloro-1-hexanol	$Cl(CH_2)_6OH$	136.62		1.204	1.4560^{20}		110^{14mm}	98	sl s aq; v s alc, eth
c151	4-Chloro-4′-hydroxybenzophenone	$ClC_6H_4C(=O)C_6H_4OH$	232.67	8[2], 187			175–178	257^{13mm}		
c152	5-Chloro-8-hydroxy-7-iodoquinoline		305.50	21, 98			172			i alc, eth; 0.8 chl; 0.6 HOAc
c153	5-Chloro-8-hydroxyquinoline		179.61	21, 95			130			sl s aq HCl
c154	1-Chloro-4-iodobenzene	ClC_6H_4I	238.46	5, 221	1.186_4^{57}		53–54	227	108	s alc
c155	1-Chloro-3-iodopropane	$Cl(CH_2)_3I$	204.44	1, 114	1.904	1.5463^{20}		170–172	>110	
c156	1-Chloro-3-mercapto-2-propanol	$HSCH_2CH(OH)CH_2Cl$	126.61	1[3], 2156	1.277	1.5276^{20}		$57^{1.3mm}$	97	
c157	Chloromethane	CH_3Cl	50.49	1, 59	2.064 g/L	1.3712^{-24}	−97.7	−24.2	<0	0.48 aq;[25] s alc,; misc chl, eth, HOAc
c158	3-Chloro-4-methoxyaniline	$ClC_6H_3(OCH_3)NH_2$	157.60	13, 511			50–55		110	
c159	5-Chloro-2-methoxyaniline	$ClC_6H_3(OCH_3)NH_2$	157.60	13, 383			83–85			
c160	1-Chloro-2-methoxybenzene	$ClC_6H_4OCH_3$	142.59	6, 184	1.123	1.5445^{20}		196	76	i aq; s alc, eth
c161	5-Chloro-2-methoxybenzoic acid	$ClC_6H_3(OCH_3)COOH$	186.59	10, 103			98–100			
c162	2-Chloro-6-methoxypyridine	$CH_3O(Cl)(C_5H_3N)$	143.57		1.207	1.5263^{20}		186		

2-Chloro-6-fluorobenzal chloride, t238
α-Chloro-4-fluorotoluene, f16
5-Chloro-2-hydroxyaniline, a147
Chlorohydroxybenzoic acids, c245, c246
1-Chloro-3-hydroxypropane, c231



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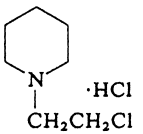

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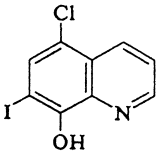

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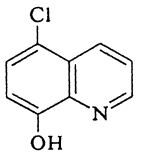


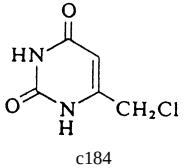
c153

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
c163	2-Chloro-6-methyl-aniline	$CH_3O(Cl)C_6H_3NH_2$	141.60	12^{1}, 388	1.152	1.5761^{20}	2	215	98	s alc
c164	3-Chloro-2-methyl-aniline	$CH_3O(Cl)C_6H_3NH_2$	141.60	12, 836	1.185	1.5874^{20}	2	117^{10mm}	>110	
c165	3-Chloro-4-methyl-aniline	$CH_3O(Cl)C_6H_3NH_2$	141.60	12, 988		1.5830^{20}	25	238	100	
c166	4-Chloro-2-methyl-aniline	$CH_3O(Cl)C_6H_3NH_2$	141.60	12, 835		1.5848^{20}	27	241	99	s hot alc
c167	5-Chloro-2-methyl-aniline	$CH_3O(Cl)C_6H_3NH_2$	141.60	12, 835		1.5840^{20}	22	237	160	
c168	3-(Chloromethyl)-benzoyl chloride	$ClCH_2C_6H_4COCl$	189.04	9^{2}, 325	1.330	1.5748^{20}		150^{20mm}	>110	
c169	**DL**-4-Chloro-2-(α-methylbenzyl)phenol	$C_6H_5CH(CH_3)C_6H_3(Cl)OH$	232.71	6^{4}, 4710	1.238	1.5994^{20}		155^{2mm}	>110	
c169a	1-Chloro-3-methyl-butane	$ClCH_2CH_2CH(CH_3)CH_3$	106.60		0.8750^{20}	1.4084^{20}	−104	99	<21	sl s aq; misc alc, eth
c170	2-Chloro-2-methyl-butane	$CH_3CH_2CCl(CH_3)_2$	106.59	1, 134	0.8650^{20}_{4}	1.4052^{20}	−73.7	85	−9	i aq; s alc, eth
c171	Chloromethyldichloro-methylsilane	$ClCH_2Si(Cl)_2CH_3$	163.5	4^{3}, 1888	1.286	1.4494^{20}		121	110	
c172	Chloromethyl ethyl ether	$ClCH_2OCH_2CH_3$	94.54	1^{2}, 645	1.04^{20}_{4}	1.4040^{20}		79–83	19	s alc; v s eth
c172a	3-(Chloromethyl)-heptane	$CH_3CH_2CH_2CH_2CH(CH_2Cl)$-$CH_2CH_3$	148.68		0.8769^{20}	1.4319^{20}		172	60	
c173	Chloromethyl methyl ether	$ClCH_2OCH_3$	80.51	1, 580	1.0703^{20}_{4}	1.3961^{20}	−103.5	57–59	15	dec by aq; s acet, CS_2
c174	Chloromethyl methyl sulfide	$ClCH_2SCH_3$	95.48		1.153	1.4963^{20}		105	17	
c175	1-(Chloromethyl)-naphthalene	$C_{10}H_7CH_2Cl$	176.65	5, 566	1.180	1.6380^{20}	32	169^{25mm}	>110	
c176	4-Chloro-2-methyl-phenol	$CH_3(Cl)C_6H_3OH$	142.59	6, 359			45–48	220–225	>110	sl s aq

c177	4-Chloro-3-methyl-phenol	$CH_3(Cl)C_6H_3OH$	142.59	6, 381			65–68	235		i aq; s alc, bz, chl, eth, acet
c178	1-Chloro-2-methyl-2-phenylpropane	$C_6H_5C(CH_3)_2CH_2Cl$	168.67	5^2, 320	1.047	1.5240^{20}		96^{10mm}	92	
c179	1-Chloro-2-methyl-propane	$(CH_3)_2CHCH_2Cl$	92.57	1, 124	0.8829^{15}	1.4010^{15}	−130.3	68.9	<21	0.09 aq; misc alc, eth
c180	2-Chloro-2-methyl-propane	$(CH_3)_3CCl$	92.57	1, 125	0.8420^{20}	1.3856^{20}	−26	50.8	<0	sl s aq; misc alc, eth
c181	1-Chloro-2-methyl-propene	$(CH_3)_2C{=}CHCl$	90.55	1, 209	0.9186^{20}_4	1.4225^{20}		68.1	−1	misc alc, eth
c182	3-Chloro-2-methyl-propene	$ClCH_2C(CH_3){=}CH_2$	90.55	1, 209	0.9210^{15}_4	1.4272^{20}	−80	72	−12	misc alc, eth
c183	Chloromethyltri-methylsilane	$ClCH_2Si(CH_3)_3$	122.67	4^3, 1844	0.8861^{20}_4	1.4180^{20}		99	−2	
c184	6-(Chloromethyl)-uracil		160.56	23^1, 328			257 dec			
c185	1-Chloronaphthalene	$C_{10}H_7Cl$	162.62	5, 541	1.1938^{20}_4	1.6326^{20}	−2.3	259	121	s alc, bz, PE
c186	2-Chloronaphthalene	$C_{10}H_7Cl$	162.62		1.1377^{71}	1.6079^{71}	60	256		s alc, bz, chl, eth
c187	4′-Chloro-3′-nitro-acetophenone	$ClC_6H_3(NO_2)C(=O)CH_3$	199.60	7^3, 995			101			
c188	2-Chloro-4-nitro-aniline	$ClC_6H_3(NO_2)NH_2$	172.57	12, 733			107–109			sl s aq; v s alc, eth
c189	2-Chloro-5-nitro-aniline	$ClC_6H_3(NO_2)NH_2$	172.57	12, 732			119–121			
c190	4-Chloro-2-nitro-aniline	$ClC_6H_3(NO_2)NH_2$	172.57	12, 729			117–119			v s alc, eth

Chloromethylbenzenes, b90, c255, c256, c257
(Chloromethyl)oxirane, c120
α-Chloronitrotoluene, n45
Chloronitro-α,α,α-trifluorotoluenes, c199, c200



c184

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
c191	4-Chloro-3-nitro-aniline	$ClC_6H_3(NO_2)NH_2$	172.57	12, 731			99–101			v s alc; s eth
c192	1-Chloro-2-nitro-benzene	$ClC_6H_4NO_2$	157.56	5, 241	1.348		33	246	123	s alc, bz, eth
c193	1-Chloro-3-nitro-benzene	$ClC_6H_4NO_2$	157.56	5, 243	1.534_4^{20}		44	236	103	sl s alc; v s chl, eth
c194	1-Chloro-4-nitro-benzene	$ClC_6H_4NO_2$	157.56	5, 243	1.520		83–84	242	>110	sl s alc; v s eth, CS_2
c195	2-Chloro-4-nitro-benzoic acid	$ClC_6H_3(NO_2)COOH$	201.57	9, 404			139–141			s hot aq, hot bz
c196	2-Chloro-5-nitro-benzoic acid	$ClC_6H_3(NO_2)COOH$	201.57	9, 403	1.608^{18}		166–168			sl s aq; s alc, bz, eth
c197	4-Chloro-3-nitro-benzoic acid	$ClC_6H_3(NO_2)COOH$	201.57	9, 402	1.645^{18}		180–183			sl s alc; s hot aq
c198	4-Chloro-3-nitro-benzophenone	$ClC_6H_3(NO_2)C(=O)C_6H_5$	261.66	7[1], 230			104–106	235^{13mm}		
c199	2-Chloro-5-nitro-benzotrifluoride	$ClC_6H_3(NO_2)CF_3$	225.55		1.527	1.5083^{20}		231	98	
c200	4-Chloro-3-nitro-benzotrifluoride	$ClC_6H_3(NO_2)CF_3$	225.55		1.511	1.4893^{20}	−2.5	222	101	
c201	4-Chloro-2-nitrophenol	$ClC_6H_3(NO_2)OH$	173.56	6, 238			85–87			
c202	2-Chloro-6-nitro-toluene	$ClC_6H_3(NO_2)CH_3$	171.58	5, 327		1.5377^{70}	36	238	125	i aq
c203	4-Chloro-2-nitro-toluene	$ClC_6H_3(NO_2)CH_3$	171.58	5, 327			39	240^{718mm}	>110	i aq
c203a	1-Chlorooctadecane	$CH_3(CH_2)_{17}Cl$	288.95	1[3], 566	0.849	1.4516^{20}		$158^{1.5mm}$	>110	
c204	1-Chlorooctane	$CH_3(CH_2)_7Cl$	148.68	1, 159	0.875	1.4298^{20}	−58	182	70	0.02 aq; misc alc, eth
c204a	1-Chloropentane	$CH_3(CH_2)_4Cl$	106.60	1, 130	0.8820^{20}	1.4115^{20}	−99	107–108	13	
c205	3-Chloro-2,4-pentane-dione	$CH_3COCH(Cl)COCH_3$	134.56	1, 785	1.129	1.4830^{20}		52^{18mm}	12	
c206	5-Chloro-2-pentanone	$ClCH_2CH_2CH_2COCH_3$	120.58	1[2], 738	1.0571_4^{18}	1.4390^{20}		72^{20mm}	35	s acet, eth
c207	3-Chloroperoxy-benzoic acid	$ClC_6H_5C(O)OOH$	172.57	9[4], 972			69–71			

c208	2-Chlorophenol	ClC_6H_4OH	128.56	6, 183	1.2573_4^{23}	1.5565^{20}	9.8	175	63	sl s aq; v s alc, eth, caustic alkali
c209	3-Chlorophenol	ClC_6H_4OH	128.56	6, 185	1.245_4^{45}	1.5565^{40}	33	214	>110	sl s aq; s alc, eth
c210	4-Chlorophenol	ClC_6H_4OH	128.56	6, 186	1.2238_4^{78}	1.5479^{40}	43	220	115	sl s aq; v s alc, chl, eth, $CHCl_3$, glyc
c211	4-Chlorophenoxyacetic acid	$ClC_6H_4OCH_2COOH$	186.59	6, 187			157–159			s aq; MeOH
c212	2-(4-Chlorophenoxy)-2-methylpropanoic acid	$ClC_6H_4OC(CH_3)_2COOH$	214.65	Merck: 12, 2437			118–119			
c213	(±)-2-(4-Chlorophenoxy)propanoic acid	$ClC_6H_4OCH(CH_3)COOH$	200.62	6^3, 695			117			
c214	4-Chlorophenylacetic acid	$ClC_6H_4CH_2COOH$	170.60	9, 448			108			v s aq, alc, eth; s bz
c215	(4-Chlorophenyl)-acetonitrile	$ClC_6H_4CH_2CN$	151.60	9, 448			30.5	265–267	>110	
c216	2-Chloro-1,4-phenylenediamine sulfate	$H_2NC_6H_3(Cl)NH_2 \cdot H_2SO_4$	240.67	13, 117			251–253			s aq
c217	4-Chloro-1,2-phenylenediamine	$ClC_6H_3(NH_2)_2$	142.59	13, 25			70–73			s mineral acids
c218	1-(4-Chlorophenyl)-ethanol	$ClC_6H_4CH(CH_3)OH$	156.61	6^1, 236	1.171	$1.541O^{20}$		119^{10mm}	>110	
c219	3-Chlorophenyl isocyanate	ClC_6H_4NCO	153.57	12, 606	1.260	1.5576^{20}	−4.4	114^{43mm}	86	
c220	4-Chlorophenyl isocyanate	ClC_6H_4NCO	153.57	12, 616	1.200	1.5618^{20}	29–31	204	>110	
c221	4-Chlorophenyl phenyl sulfone	$ClC_6H_4SO_2C_6H_5$	252.72	6^1, 149			94			at 20°C: 74 acet; 44 bz; 5 CCl_4; 65 diox; 21 i-PrOH
c222	1-Chloro-3-phenylpropane	$C_6H_5(CH_2)_3Cl$	154.64	5, 391	1.080	1.5207^{20}		219	87	
c223	4-Chlorophenyl sulfone	$(ClC_6H_5)_2SO_2$	287.17	6, 327			145–148	250^{10mm}		

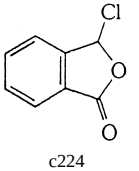
p-Chlorophenacyl bromide, b286
Chlorophenylamines, c38, c39, c40
4-Chlorophenyl sulfone, b171
4-Chlorophenyl sulfoxide, b172

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
c224	3-Chlorophthalide		168.58	17^{1}, 162			58	150^{10mm}		
c225	1-Chloropropane	$CH_3CH_2CH_2Cl$	78.54	1, 104	0.8899^{20}	1.3886^{20}	−122.8	46–47	−31	0.27 aq; misc alc, eth
c226	2-Chloropropane	$CH_3CHClCH_3$	78.54	1, 105	0.8563^{20}	1.3777^{20}	−117	35–36	−35	0.2 aq[20]; misc alc, bz, chl, eth
c227	3-Chloro-1,2-propanediol	$ClCH_2CH(OH)CH_2OH$	110.54	1, 473	1.3218_4^{20}	1.4805^{20}		213	>110	s aq, alc, eth
c228	2-Chloropropanoic acid	$CH_3CH(Cl)COOH$	108.52	2, 248	1.182	1.4345^{20}		170–190	101	misc aq, alc, eth
c229	3-Chloropropanoic acid	$ClCH_2CH_2COOH$	108.52	2, 249			41	200^{765mm}	>110	v s aq, alc, chl; s eth
c230	1-Chloro-2-propanol	$CH_3CH(OH)CH_2Cl$	94.54	1, 363	1.115^{20}	1.4375_4^{20}		126–127	51	misc aq; s alc
c231	3-Chloro-1-propanol	$ClCH_2CH_2CH_2OH$	94.54	1, 356	1.1309_4^{20}	1.4450^{20}		160–162	73	
c232	Chloro-2-propanone	$ClCH_2COCH_3$	92.53	1, 653	1.135^{15}	1.4320^{20}	−44.5	119.7	27	10 aq; misc alc, chl, eth
c233	3-Chloropropanonitrile	$ClCH_2CH_2CN$	89.53	2, 250	1.1443^{18}	1.4341^{20}	−51	95^{50mm} d > 130	75	
c234	3′-Chloropropanophenone	$ClC_6H_4C(=O)CH_2CH_3$	168.62	7^{3}, 1028			45–47	124^{14mm}	>110	
c235	2-Chloropropanyl chloride	$CH_3CH(Cl)COCl$	126.97	2, 248	1.308	1.4400^{20}		109–111	31	dec aq, alc
c236	3-Chloropropanyl chloride	$ClCH_2CH_2COCl$	126.97	2, 250	1.3307^{13}	1.4570^{20}		143–145	61	i aq; d hot aq, hot alc; s alc; v s eth
c236a	3-Chloro-1-propene	$ClCH_2CH{=}CH_2$	76.53	1, 198	0.938_4^{20}	1.4154^{20}	−134.5	45	−32	0.36 aq; misc alc, PE
c237	3-Chloropropylacetate	$CH_3CO_2(CH_3)_3Cl$	130.02	4, 148			148–150			
c238	3-Chloropropyl thiolactate	$CH_3C(=O)SCH_2CH_2Cl$	152.64	2^{3}, 493	1.159	1.4946^{20}		84^{10mm}	77	
c239	(3-Chloropropyl)triethoxysilane	$Cl(CH_2)_3Si(OC_2H_5)_3$	240.81		1.009_4^{20}	1.420^{20}		102^{10mm}		
c240	(3-Chloropropyl)trimethoxysilane	$Cl(CH_2)_3Si(OCH_3)_3$	198.72		1.077_4^{25}	1.4183^{25}		195^{750mm}	78	
c241	3-Chloropropyne	$ClCH_2C{\equiv}CH$	74.51	1, 248	1.0306_4^{25}	1.4560^{20}	−78	57	−13	misc alc, bz, eth, EtOAc
c242	2-Chloropyridine	$Cl(C_5H_4N)$	113.55	20, 230	1.205^{15}	1.5320^{20}		166^{714mm}	65	sl s aq; s alc, eth

c243	3-Chloropyridine	$Cl(C_5H_4N)$	113.55	20, 230	1.194	1.5300^{20}		148	65	
c244	4-Chlororesorcinol	ClC_6H_3-1,3$(OH)_2$	144.56	6^2, 818			106–108	147^{18mm}		
c245	4-Chlorosalicylic acid	ClC_6H_3(2-OH)COOH	172.57	10, 101			210–212			
c246	5-Chlorosalicylic acid	ClC_6H_3(2-OH)COOH	172.57	10, 102			172			
c247	*N*-Chlorosuccinimide		133.53	21, 380	1.65		150–151			1.4 aq; 0.67 alc; 2 bz; sl s chl, CCl_4, eth
c248	Chlorosulfonic acid	$ClHO_3S$	116.52	Merck: 12, 2218	1.753_4^{20}	1.437^{14}	−80	152^{755mm}	none	s pyr, dichloroethane; aq dec with violence
c249	Chlorosulfonyl isocyanate	$ClSO_2NCO$	141.53		1.626	1.4470^{20}	−44	107	none	
c250	1-Chlorotetradecane	$CH_3(CH_2)_{13}Cl$	232.84	1^2, 135	0.859	1.4460^{20}		142^{4mm}	>110	
c251	2-Chlorothiophene	$Cl(C_5H_3S)$	118.59	17, 32	1.286	1.5483^{20}	−72	127–129	22	i aq; misc alc, eth
c252	4-Chlorothiophenol	ClC_6H_4SH	144.62	6, 326			49–52	205–207	>110	
c253	8-Chlorothiophylline		214.61	26, 473			dec 290			s alkali
c254	Chlorotitanium triisopropoxide	$[(CH_3)_2CHO]_3TiCl$	260.62		1.091				22	
c255	2-Chlorotoluene	$ClC_6H_4CH_3$	126.59	5, 290	1.0826_4^{20}	1.5268^{20}	−35.6	159.0	47	sl s aq; v s alc, bz, chl, eth
c256	3-Chlorotoluene	$ClC_6H_4CH_3$	126.59	5, 291	1.0760_4^{19}	1.5218^{20}	−47.8	161.8	50	s alc, bz, chl; misc eth
c257	4-Chlorotoluene	$ClC_6H_4CH_3$	126.59	5, 292	1.0697_4^{20}	1.5150^{20}	7.5	162.4	49	sl s aq; s alc, bz, eth
c258	*N*-Chloro-*p*-toluene sulfonamide, sodium salt	$CH_3C_6H_4SO_2NCl^-\ Na^+$	227.67				167 dec			s aq; i bz, chl, eth
c259	4-(4-Chloro-*o*-tolyloxy)butyric acid	$ClC_6H_3(CH_3)O(CH_2)_3COOH$	228.68				99–100			

Chloroprene, c236a
3-Chloropropylene-1,2-oxide, c120
α-Chlorotoluene, b90
β-Chloropropionaldehyde diethyl acetal, c97
1-Chloro-2,5-pyrrolidinedione, c247
Chlorotoluidines, c163 thru c167



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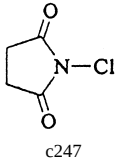

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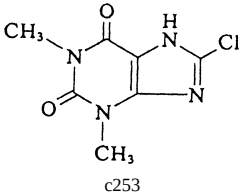

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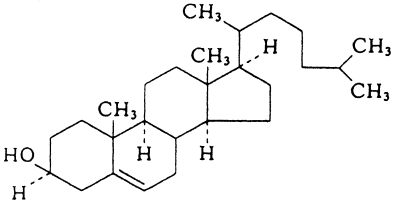
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
c260	Chlorotriethylgermane	$(C_2H_5)_3GeCl$	195.23	4^3, 1912	1.175	1.4590^{20}			>110	
c261	Chlorotriethylsilane	$(C_2H_5)_3SiCl$	150.73	4, 624	0.898	1.4300^{20}		142–144	29	
c262	Chloro-2,2,2-trifluoro-ethane	CF_3CH_2Cl	118.5	1,*3*, 138	1.389^{0}	1.3090^{0}	−105	6.9		
c263	Chlorotrifluoro-ethylene	$CF_2{=}CFCl$	116.47	1^3, 646	1.315		−158.2	−28		
c264	Chlorotrifluoro-methane	$ClCF_3$	104.46	1^3, 42	4.270 g/L		−181	−81		
c265	Chlorotrimethyl-germane	$(CH_3)_3GeCl$	153.16		1.2382^{22}	1.4283^{20}	−13	102	1	
c266	Chlorotrimethylsilane	$(CH_3)_3SiCl$	108.64	4,*3*, 1857	0.8580_4^{20}	1.3870^{20}	−40	57	−27	
c267	Chlorotriphenyl-methane	$(C_6H_5)_3CCl$	278.78	5, 700			110–112	235^{20mm}		v s bz, chl, eth
c268	Chlorotriphenyltin	$(C_6H_5)_3SnCl$	385.46	12, 914			108 dec	240^{14mm}		
c268a	Chloro-tris(dimethyl-amino)silane	$[(CH_3)_2N]_3SiCl$	195.8		0.975_4^{20}	1.442^{20}		63^{12mm}		
c269	α-Chloro-*o*-xylene	$CH_3C_6H_4CH_2Cl$	140.61	5, 364	1.063	1.5391^{20}		96^{25mm}	73	i aq; misc alc, eth
c270	α-Chloro-*m*-xylene	$CH_3C_6H_4CH_2Cl$	140.61	5, 373	1.064^{20}	1.5350^{20}		195–196	75	i aq; misc alc, eth
c271	α-Chloro-*p*-xylene	$CH_3C_6H_4CH_2Cl$	140.61	5, 384		1.5330^{20}	4.5	200	75	misc alc, bz, eth, acet
c272	2-Chloro-*p*-xylene	$ClC_6H_3(CH_3)_2$	140.61	5, 384	1.049	1.5240^{20}	2	186	57	
c273	4-Chloro-*p*-xylene	$ClC_6H_3(CH_3)_2$	140.61	5, 363	1.047	1.5280^{20}		221–223	66	misc alc, bz, eth, acet
c274	Cholesterol		386.66	6,*3*, 2607	1.052_{19}^{19}		148.5	$203^{0.5mm}$		1.3 alc; 35 eth; 22 chl; s bz, PE
c275	Cholic acid		408.58	10^3, 2162			198			(15°): 0.03 aq; 3.1 alc; 2.8 acet; 15.2 HOAc; 0.5 chl; 0.036 bz
c276	Cinchonine		194.40	23^2, 369			ca. 260			1.6 alc; 0.9 chl; 0.2 eth
c277	1,8-Cineole		154.25	17, 23	0.921_{25}^{25}	$1,4572^{20}$	1	176.4	48	misc alc, chl, eth
c278	*trans*-Cinnamaldehyde	$C_6H_5CH{=}CHCHO$	132.16	7, 348	1.050_{25}^{25}	1.6219^{20}	−7.5	136^{20mm}	71	0.014 aq; misc alc, chl, eth
c279	*trans*-Cinnamic acid	$C_6H_5CH{=}CHCOOH$	148.16	9, 573	1.2475_4^4		133	300		0.05 aq; 16 alc; 8 chl

c280	*trans*-Cinnamoyl chloride	$C_6H_5CH{=}CHCOCl$	166.61	9[2], 390	1.1617^{25}_{4}	1.614^{43}	35–36	258	>110	s hot alc, CCl_4
c281	Cinnamyl acetate	$CH_3CO_2CH_2CH{=}CHC_6H_5$	176.22	6[2], 527	1.0571	1.5421^{20}		265	>110	
c282	Cinnamyl alcohol	$C_6H_5CH{=}CHCH_2OH$	134.18	6, 570	1.0397^{35}_{35}	1.5758^{33}	33	250.0	>110	s aq; v s common organic solvents
c283	Cinnamyl chloride	$C_6H_5CH{=}CHCH_2Cl$	159.62	5, 482	1.096	1.5840^{20}	−19	108^{12mm}	79	
c284	Citraconic acid	$CH_3C(COOH){=}CHCOOH$	130.10	2, 768	1.62		92 dec			v s aq, alc, eth; sl s chl; i bz, PE
c285	Citraconic anhydride		112.08	17, 440	1.247	1.4712^{20}	8	214	101	
c286	Citral (geranial plus neral, *cis* and *trans* forms, resp.)	$(CH_3)_2C{=}CHCH_2CH_2$-$C(CH_3){=}CHCHO$	152.24		0.888	1.4876^{20}		229	101	

2-Chlorotriethylamine, d328
2-Chloro-2-(trifluoromethyl)aniline, a141
Chloro-α,α,α-trifluorotoluenes, c60, c61, c62
4-Chloro-α,α,α-trifluoro-*o*-toluidine, a142
α'-Chloro-α,α,α-trifluoro-*m*-xylene, t304
Chlorotrihexylsilane, t307
Chloroxylenol, c109
Chromone, b55
Chrysene, b52
Cinchophen, p153
Citral, d644, d645



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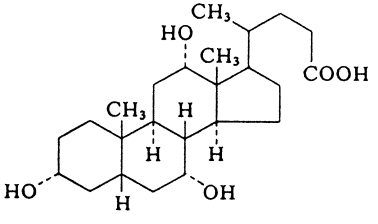

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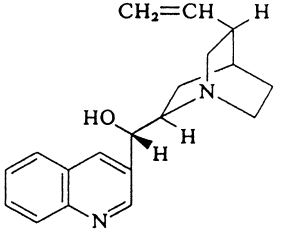

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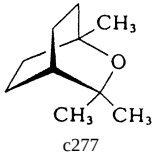

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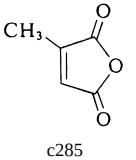


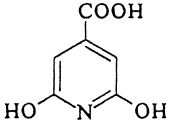
c285

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

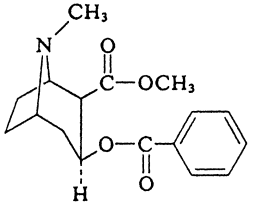
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
c287	Citral dimethyl acetal	$(CH_3)_2C{=}CHCH_2CH_2$-$C(CH_3){=}CH(OCH_3)_2$	198.31	1^4, 3570	0.890	1.4540^{20}		106^{10mm}	92	
c288	Citrazinic acid		155.11	22, 254			carbonizes without melting >300			i aq; s alkali
c289	Citric acid	$HOOCCH_2C(OH)(COOH)$-CH_2COOH	192.12	3, 556	1.665		154			59 aq
c290	*β*-Citronellol	$(CH_3)_2C{=}CHCH_2CH_2$-$CH(CH_3)CH_2CH_2OH$	156.27	1^1, 232	0.8570_4^{20}	1.4560^{20}		222	98	v sl s aq; misc alc, eth
c299	Cocaine		303.35	22^2, 150		1.5022^{98}	98	$187^{0.1mm}$		0.17 aq; 15 alc; 140 chl; 28 eth; s acet; EtOAc, CS_2
c300	Coumarin		146.15	17, 328	0.935_4^{20}		68–70	298		0.25 aq; v s alc, chl, eth; s alkali
c301	Creatine	$HOOCCH_2N(CH_3)$-$C(=NH)NH_2$	131.14	4, 363			dec 303			1.3 aq; 0.11 alc; i eth
c302	Creatinine		113.12	24, 245			255 dec			8 aq; sl s alc; i eth
c303	*o*-Cresol	$CH_3C_6H_4OH$	108.14	6, 349	1.0273^{41}	1.5361^{41}	30	191	81	$3.1\ aq^{40}$; misc alc, chl, eth; s alkali
c304	*m*-Cresol	$CH_3C_6H_4OH$	108.14	6, 373	1.034_4^{20}	1.5438^{20}	12	202.2	86	$2.5\ aq^{40}$; misc alc, chl, eth; s alkali
c305	*p*-Cresol	$CH_3C_6H_4OH$	108.14	6, 389	1.0179^{41}	1.5312^{41}	34.8	201.9	86	$2.3\ aq^{40}$; misc alc, chl, eth; s alkali
c306	*trans*-Crotonaldehyde	$CH_3CH{=}CHCHO$	70.09	1, 728	0.8516^{20}	1.4373^{20}	−76	102–104	13	$18.1\ aq^{20}$
c307	Crotonic acid	$CH_3CH{=}CHCOOH$	86.19	2, 408	0.964_4^8	1.4228^{80}	71.6	185	87	$54.6\ aq^{20}$; 52.5 $EtOH^{25}$; 53 acet; 37.5 toluene
c308	Crotonic anhydride	$(CH_3CH{=}CHO)_2O$	154.17	2, 411	1.040	1.4740^{20}		248	110	
c309	Crotononitrile	$CH_3CH{=}CHCN$	67.09	2, 412	1.4190^{20}	1.4190^{20}		121	20	
c310	Crotonyl chloride	$CH_3CH{=}CHCOCl$	104.54	2, 411	1.091	1.4600^{20}		120–123	35	
c311	Crotyl alcohol	$CH_3CH{=}CHCH_2OH$	72.11	1, 442	0.845	1.4270^{20}		122	37	17 aq; misc alc
c312	Crotyl chloride	$CH_3CH{=}CHCH_2Cl$	90.55	1^2, 176	0.929	1.4360^{20}		85	−5	
c313	12-Crown-4		176.21		1.089	1.4630^{20}		$70^{0.5mm}$	>110	specific for Li^+

c314	18-Crown-6		264.32				42–45		>110
c315	Crystal Violet		407.99	13, 756			215 dec		
c316	Cumene hydro-peroxide	$C_6H_5C(CH_3)_2OH$	152.20	6^3, 1814	1.030	1.5210^{20}		101^{8mm}	56

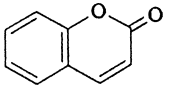
Cleland's reagent, d484
2,4,6-Collidine, t393
p-Coumaric acid, h109
Cresylic acids, c303, c304, c305
trans-Crotonic acid, b484
Crotononitrile, b482
trans-Crotonyl alcohol, c311
Crotyl alcohols, b486, b487
Crotyl bromide, b276
Crotyl chloride, c79
12-Crown-4, t124
15-Crown-5, p46
Cumene, i103
Cumic alcohol, i104



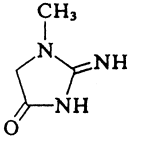
c288



c299



c300



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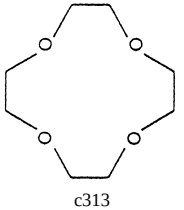

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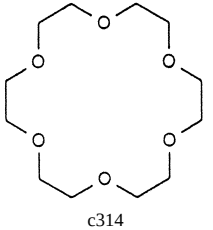

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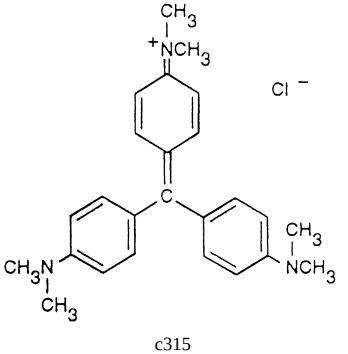


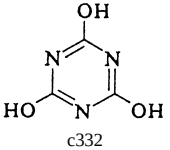
c315

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
c316a	Cumylphenol	$C_6H_5C(CH_3)_2C_6H_4OH$	212.29				74–76	335		
c317	Cupferron	$C_6H_5N(NO)O^- NH_4^+$	155.16	16^1, 395			163–164			v s aq, alc
c318	Cyanamide	H_2NCN	42.04	3^2, 63	1.282_4^{20}		46	83^{380mm}	>110	78 aq; 29 BuOH; 42 EtOAc; s alc, eth
c319	2-Cyanoacetamide	$NCCH_2CONH_2$	84.08	2, 589			119.5		215	25 aq; 3.1 alc
c320	Cyanoacetic acid	$NCCH_2COOH$	85.06	2, 583			66	108^{15mm}	107	s aq, alc, eth; sl s bz
c321	Cyanoacetohydrazide	$NCCH_2C(=O)NHNH_2$	99.09	Merck: 11, 2688			115	dec		v s aq; s alc; i eth
c322	Cyanoacetylurea	$NCCH_2C(=O)NH$-$C(=O)NH_2$	127.10	3, 66			214 dec			
c323	2-Cyanoethanol	$NCCH_2CH_2OH$	71.08	3^2, 213	1.0588^0			108^{11mm}		misc aq, alc; sl s eth
c324	2-Cyanoethyl acrylate	$H_2C{=}CHCO_2CH_2CH_2CN$	125.13	3^3, 543	1.052	1.4470^{20}		108^{12mm}	103	
c325	Cyanogen bromide	BrCN	105.93	3, 39	2.015_4^{20}		52	61–62	5	v s aq, alc, eth
c326	1-Cyano-3-methyliso-thiourea, sodium salt	$CH_2NH(=NCN)S^- Na^+$	137.14	4, 71			290 dec			
c327	1-Cyanonaphthalene	$C_{10}H_7CN$	153.18	9, 649	1.1113_{25}^{25}	1.6298^{18}	38	299		i aq; v s alc, eth
c328	2-Cyanopyridine	$NC(C_5H_4N)$	104.11	22, 36	1.081	1.5288^{20}	26–28	215	89	s aq; v s alc, bz, eth
c329	3-Cyanopyridine	$NC(C_5H_4N)$	104.11	22, 41			50–52	201	84	v s aq, alc, bz, eth
c330	4-Cyanopyridine	$NC(C_5H_4N)$	104.11	22, 46			78–80			s aq, alc, bz, eth
c331	Cyanotrimethylsilane	$(CH_3)_3SiCN$	99.21	4^4, 3893	0.783_4^{20}	1.3924^{20}	11–12	118–119	1	
c332	Cyanuric acid		129.08	26, 239	1.768^0		>360; dec to HOCN			0.5 aq; s hot alc, pyr; i acet, bz, chl, eth
c333	Cyclobutane	C_4H_8	56.10	5, 17	0.7038^0	1.3752^0	−91	13		i aq; v s alc, acet
c334	Cyclobutanecarboxylic acid	$(C_4H_7)COOH$	100.12	9, 5	1.047	1.4433^{20}	−20 to −7.5	195	83	
c335	Cyclodecane	$C_{10}H_{20}$	140.27		0.871	1.4707^{20}		201	65	
c336	Cyclododecanol	$C_{12}H_{23}OH$	184.32				77			
c337	Cyclododecanone	$C_{12}H_{22}(=O)$	182.31	7^2, 48	0.906^{62}		59–61	85^{1mm}		
c338	*trans,trans,cis*-1,5,9-cyclododecatriene		162.28	5^4, 1115	0.8925_4^{20}	1.5070^{20}	−18	231	87	
c339	Cyclododecene		166.31		0.863	1.4822^{20}		232–245	93	
c340	Cyclododecylamine	$(C_{12}H_{23})NH_2$	183.34				28–30	124^{7mm}	121	

c341	Cycloheptane	C_7H_{14}	98.18	5, 29	0.811_4^{20}	1.4455^{20}	−8.0	118	6	v s alc, eth
c342	Cycloheptanol	$C_7H_{13}OH$	114.19	6, 10	0.948_4^{20}	1.4760^{20}	2	185	71	sl s aq; v s alc, eth
c343	Cycloheptanone	$C_7H_{12}(=O)$	112.17	7, 13	0.9490_4^{20}	1.4611^{20}		179–181	55	i aq; v s alc; s eth
c344	1,3,5-Cycloheptatriene		92.13	5, 280	0.888	1.5211^{20}	−75.3	115.5	26	s alc, eth; v s bz, chl
c345	Cycloheptene	C_7H_{12}	96.17	5, 65	0.824	1.4585^{20}		114.7	−6	s alc, eth
c346	8-Cyclohexadecene-1-one		236.40	7[3], 521		1.4890^{20}		195^{19mm}	>110	
c347	Cyclohexane	C_6H_{12}	84.16	5, 20	0.7786_4^{20}	1.4262^{20}	6.6	80.7	−20	0.01 aq; misc acet, alc, bz, CCl_4, eth
c348	Cyclohexane-d_{12}	C_6D_{12}	92.26	5[3], 36	0.893	1.4210^{20}		78	−18	
c349	1,3-Cyclohexanebis(methylamine)	$C_{10}H_{10}(NHCH_3)_2$	142.25		0.945	1.4930^{20}			106	
c350	1,3-Cyclohexanecarbonitrile	$C_6H_{11}CN$	109.17	9, 9	0.919	1.4505^{20}		76^{16mm}	65	
c351	Cyclohexanecarbonyl chloride	$C_6H_{11}COCl$	146.62	9, 9	1.096	1.4700^{20}		184	66	
c352	Cyclohexanecarboxaldehyde	$C_6H_{11}CHO$	112.17	7, 19	0.926	1.4500^{20}		163	40	

Cupron, b50
Cyanoacetonitrile, m5
Cyanoanilines, a121, a122, a123
Cyanobenzene, b51
2-Cyanoethanol, h173
Cyanoethylene, a63
Cyanomethane, a29
1-Cyanopropane, b468a
2-Cyano-1-propene, m30a
2-Cyanotoluene, t184
4-Cyanotoluene, t185
Cyanuric chloride, t255
1,5-Cyclododecadiene-9,10-epoxide, e4
Cyclododecane epoxide, e5
Cycloheptanone isooxime, a307
Cycloheptyl bromide, b310
2,5-Cyclohexadien-1,4-dione, b58
2,5-Cyclohexadiene-1,4-dione with 1,4-benzenediol (1:1), q1
Cyclohexaneacetic acid, c373



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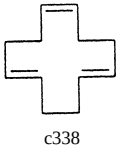
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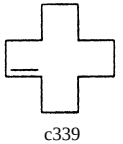
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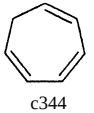
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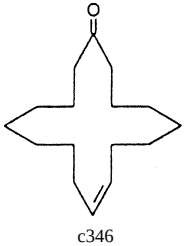


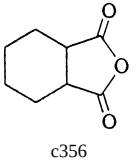
c346

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
c353	Cyclohexanecarboxylic acid	$C_6H_{11}COOH$	128.17	9, 7	1.0480^{15}_{4}	1.4530^{20}	29	232.5	>110	0.21 aq; s alc, bz, eth
c354	*trans*-1,2-Cyclohexanediamine	$C_6H_{10}(NH_2)_2$	114.19	13^3, 8	0.951	1.4884^{20}	14–15	92^{18mm}	68	
c355	1,3-Cyclohexanedicarboxylic acid	$C_6H_{10}(COOH)_2$	172.18	9, 732			132–141			
c356	*cis*-1,2-Cyclohexanedicarboxyic anhydride		154.17	17, 452			32–34	158^{17mm}	>110	
c357	1,4-Cyclohexanedimethanol	$C_6H_{10}(CH_2OH)_2$	144.21		0.978^{100}_{4}	1.4893^{20}	43	283	161	misc aq, alc; 2.5 eth
c358	1,4-Cyclohexanedivinyl ether	$C_6H_{10}(OCH{=}CH_2)_2$	196.29		0.919	1.4720^{20}		126^{14mm}	>110	
c359	1,4-Cyclohexanediol	$C_6H_{10}(OH)_2$	116.16	6, 741			98–100	150^{20mm}	65	
c360	1,3-Cyclohexanedione	$C_6H_8(=O)_2$	112.13	7, 554	1.0861^{91}	1.4576^{102}	103–105			s aq, alc, acet, chl
c361	1,2-Cyclohexanedione dioxime	$C_6H_8(=NOH)_2$	142.16	7^2, 526			185–188			s aq
c362	Cyclohexanemethylamine	$C_6H_{11}CH_2NH_2$	113.20	12, 12	0.870	1.4630^{20}		145–147	43	
c363	Cyclohexanepropionic acid	$C_6H_{11}CH_2CH_2COOH$	156.23	9, 82	0.912	1.4636^{20}	14–17	275.8	>110	
c364	Cyclohexanethiol	$C_6H_{11}SH$	116.23	6, 8	0.950	1.4921^{20}		158–160	43	
c365	Cyclohexanol	$C_6H_{11}OH$	100.16	6, 5	0.9416^{30}	1.4629^{30}	25.4	161	68	3.8 aq^{25}; misc alc, bz
c366	Cyclohexanone	$C_6H_{10}(=O)$	98.15	7, 8	0.9478^{20}_{4}	1.4510^{20}	−31	155.7	44	15 aq^{10}; s alc, eth
c367	Cyclohexanone oxime	$C_6H_{10}(=NOH)$	113.16	7, 10			89–91	206–210		s aq, eth; sl s alc
c368	Cyclohexene	C_6H_{10}	82.15	5, 63	0.8094^{20}_{4}	1.4464^{20}	−103.5	83.0	−12	0.02 aq; misc alc, bz, acet, eth
c369	3-Cyclohexene-1-methanol	$C_6H_9CH_2OH$	112.17	6^3, 215	0.961	1.4853^{20}		85^{18mm}	76	
c370	Cyclohexene oxide		98.15	17, 21	0.970	1.4520^{20}		130	27	
c371	2-Cyclohexene-1-one	$C_6H_8(=O)$	96.13	7^2, 55	0.993	1.4885^{20}	−53	168	56	v s alc
c372	4-(3-Cyclohexene-1-yl)pyridine		159.23	20^3, 3239	1.021	1.5480^{20}		141^{20mm}	>110	
c373	Cyclohexyl acetate	$CH_3CO_2C_6H_{11}$	142.20	6, 7	0.966	1.4395^{20}		173	57	sl s aq; s org solv

c374	Cyclohexylacetic acid	$C_6H_{11}CH_2COOH$	142.20	9[2], 9	1.007	1.4630^{20}	31–33	242–244	>110	
c375	Cyclohexylamine	$C_6H_{11}NH_2$	99.18	12, 5	0.8671^{20}	1.4593^{20}	−18	134	31	misc aq, alc, chl, eth
c376	Cyclohexylbenzene	$C_6H_{11}C_6H_5$	160.26	5, 503	0.9502_4^{20}	1.5258^{20}	7	240	98	i aq; v s alc, eth
c377	Cyclohexyldimethoxymethylsilane	$C_6H_{11}Si(OCH_3)_2CH_3$	188.35		0.940	1.4390^{20}		201.2	73	
c378	2-Cyclohexylethanol	$C_6H_{11}CH_2CH_2OH$	128.22	6, 17	0.919	1.4647^{20}		207^{745mm}	86	
c379	Cyclohexylethyl acetate	$CH_3CO_2CH_2CH_2C_6H_{11}$	170.25		0.949	1.4461		98^{15mm}	81	
c380	*N*-Cyclohexylformamide	$C_6H_{11}NHCHO$	127.18	12[2], 11			38–40	113^{10mm}	>110	
c381	Cyclohexyl isocyanate	$C_6H_{11}NCO$	125.17	12[2], 12	0.980	1.4551^{20}		168–170	48	
c382	Cyclohexyl isothiocyanate	$C_6H_{11}NCS$	141.24	12[2], 12	0.996	1.5350^{20}		219	95	
c383	Cyclohexyl methacrylate	$H_2C{=}C(CH_3)CO_2C_6H_{11}$	168.24	6[3], 25	0.964	1.4580^{20}		70^{4mm}	82	
c384	Cyclohexylmethanol	$C_6H_{11}CH_2OH$	114.19	6, 14	0.9215_4^{25}	1.4640^{25}		181	71	s alc, eth
c385	3-Cyclohexyl-1-propanol	$C_6H_{11}CH_2CH_2CH_2OH$	142.24	6[1], 15	1.007	1.4975^{20}		218	101	
c386	*N*-Cyclohexyl-2-pyrrolidinone		167.25	21[3], 3149	1.026	1.495	12	284	>110	

Cyclohexanecarboxylic acid chloride, c351
Cyclohexaneethanol, c378
Cyclohexaneethyl acetate, c379
Cyclohexanemethanol, c384
Cyclohexanone cyanohydrin, h112
cis-4-Cyclohexene-1,2-dicarboximide, t82
cis-4-Cyclohexene-1,2-dicarboxylic anhydride, t81
N-(1-Cyclohexen-1-yl)morpholine, m465
N-(1-Cyclohexen-1-yl)pyrrolidine, p284
Cyclohexyl alcohol, c365
Cyclohexyl bromide, b311
Cyclohexyl chloride, c91
Cyclohexyl ketone, c366
Cyclohexyl mercaptan, c364
Cyclohexylmethane, m202
Cyclohexylmethyl bromide, b367



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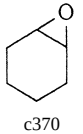

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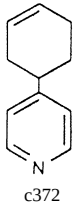

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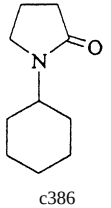

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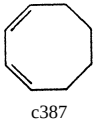
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
c387	*cis*,*cis*-1,3-Cyclooctadiene		108.18	5^{4}, 401	0.869	1.4928^{20}	−53 to −51	55^{34mm}	24	
c388	1,5-Cyclooctadiene		108.18	5, 116	0.8818^{25}_{4}	1.4905^{25}	−69	149–150	31	s CCl_4
c389	Cyclooctane	C_8H_{16}	112.22	5, 35	0.834	1.4574^{20}	14.8	151.1	30	
c390	*trans*-1,2-Cyclooctanediol	$C_8H_{14}(OH)_2$	144.21	6^{3}, 4094	1.080	1.4980^{20}	32	$94^{0.5mm}$	>110	
c391	Cyclooctanol	$C_8H_{15}OH$	128.22	6^{2}, 25	0.9740^{20}_{4}	1.4850^{20}	14–15	108^{22mm}	86	
c392	Cyclooctanone	$C_8H_{14}(=O)$	126.20	7, 21	0.9584^{20}_{4}	1.6494^{20}	41–43	195–197	72	
c393	*cis*-Cyclooctene	C_8H_{14}	110.20	5^{1}, 35	0.846	1.4698^{20}	−16	145–146	25	
c394	Cyclooctylamine	$C_8H_{15}NH_2$	127.23		0.928	1.4804^{20}	−48	190	62	
c395	Cyclopentadiene		66.10	Merck: 12, 2807	0.8021^{20}_{4}	1.4463^{16}	−85	41–42		misc alc, bz, CCl_4, eth; s aniline, HOAc, CS_2
c396	Cyclopentane	C_5H_{10}	70.13	5, 19	0.7460^{20}_{4}	1.4068^{20}	−94	49.3	−37	i aq; misc alc, eth
c397	Cyclopentanecarboxylic acid	C_5H_9COOH	114.14	9, 6	1.053^{20}_{4}	1.4540^{20}	4	216	93	sl s aq; s MeOH
c398	Cyclopentanol	C_5H_9OH	86.13	6, 5	0.9488^{20}_{4}	1.4521^{20}	−19	140	51	sl s aq; s alc
c399	Cyclopentanone	$C_5H_8(=O)$	84.12	7, 5	0.9509^{18}_{4}	1.4366^{20}	−51	130.6	26	sl s aq; misc alc, eth
c400	Cyclopentanone oxime	$C_5H_8(=NOH)$	99.13	7, 7			53–55	196	92	s aq, alc, bz, chl, eth
c401	Cyclopentene	C_5H_8	68.11	5, 61	0.7720^{20}	1.4228^{20}	−135.1	44.2	−29	
c402	2-Cyclopentene-1-acetic acid	$C_5H_7CH_2COOH$	126.16	9, 42	1.047	1.4675^{20}	19	$94^{2.5mm}$	>110	
c403	*N*-(1-Cyclopenten-1-yl)morpholine		153.23		0.957	1.5105^{20}		106^{12mm}	60	
c404	Cyclopentylamine	$C_5H_9NH_2$	85.15	12, 4	0.863	1.4482^{20}		106–108	17	
c405	3-Cyclopentylpropanoic acid	$C_5H_9CH_2CH_2COOH$	142.20		0.996	1.4570^{20}		130^{12mm}	46	
c406	Cyclopropane	C_3H_6	42.08	5, 15	0.720^{-79}_{4}		−127	−32.8		37 mL/100 mL aq[15]; v s alc, eth
c407	Cyclopropanecarbonitrile	C_3H_5CN	67.09	9, 4	0.911^{16}	1.4207^{20}		135	32	s eth
c408	Cyclopropanecarbonyl chloride	C_3H_5COCl	104.54	9, 4	1.152	1.4522^{20}		119	23	

c409	Cyclopropane-carboxylic acid	C_3H_5COOH	86.09	9, 4	1.088	1.4380^{20}	17–19	182–184	71	sl s hot aq; s alc, eth
c410	Cyclopropyl methyl ketone	$C_3H_5COCH_3$	84.12	7, 7	0.8993^{20}_4	1.4240^{20}		114	21	s aq, alc, eth
c411	L-Cysteine	$HSCH_2CH(NH_2)COOH$	121.16	4, 506			220 dec			v s aq, alc; i bz, eth
c412	L-Cystine	$HOOCCH(NH_2)SSCH_2$-$CH(NH_2)COOH$	240.30	4, 507			dec 240			0.01 aq; s acid, alkali; i alc
d1	1,9-Decalene	$H_2C{=}CH(CH_2)_6CH{=}CH_2$	138.25	1[1], 123	0.750	1.4320^{20}		169	41	
d2	*cis*-Decahydro-naphthalene	$C_{10}H_{18}$	138.25	5, 92	0.8963^{20}_4	1.4810^{20}	−43	195.8	58 (CC)	v s alc, chl, eth; misc most ketones, esters
d3	*trans*-Decahydro-naphthalene	$C_{10}H_{18}$	138.25	5[2], 56	0.8700^{20}_4	1.4690^{20}	−30.4	187.3	54	see under *cis*
d4	Decahydro-2-naphthol	$C_{10}H_{17}OH$	154.25	6, 67	0.996	1.500^{20}		109^{14mm}	>110	
d5	Decamethylcyclo-pentasiloxane	$[—Si(CH_3)_2O—]_5$	370.78	4[4], 4128	0.9593^{20}_4	1.3982^{20}	−38	101^{20mm}	72	i aq
d6	Decamethyltetra-siloxane	$(CH_3)_3SiO[Si(CH_3)_2O]_2$-$Si(CH_3)_3$	310.69	4[3], 1879	0.8536^{20}_4	1.3895^{20}	−68	194	62	sl s alc; s bz, PE
d7	Decanal	$H(CH_2)_9CHO$	156.27	1, 711	0.830^{15}_4	1.4280^{20}	−5	208–209	85	i aq; s alc, eth
d8	Decane	$CH_3(CH_2)_8CH_3$	142.29	1, 168	0.7301^{20}_4	1.4110^{20}	−29.7	174.1	46	0.07 aq
d9	1,10-Decanediamine	$H_2N(CH_2)_{10}NH_2$	172.32	4, 273			62–63	140^{12mm}		
d10	Decanedioic acid	$HOOC(CH_2)_8COOH$	202.25	2, 718	1.207^{20}_4	1.422^{134}	134.5	232^{10mm}		0.1 aq[20], eth[17]; v s alc, esters, ketones
d11	1,2-Decanediol	$CH_3(CH_2)_7CH(OH)CH_2OH$	174.28	1, 494			48–50	255	>110	
d12	1,10-Decanediol	$HO(CH_2)_{10}OH$	174.28	1[2], 560			74	170^{8mm}	>110	sl s aq, eth; v s alc

Cyclopentanepropanoic acid, c405
Cyclopentene oxide, e42
Cyclopentyl bromide, b313
Cyclopentyl chloride, c93
Cyclopropyl bromide, b314
Cyclopropyl cyanide, c407
Cymenes, i118 thru i120
Cysteamine, a161
Cytosine, a194
p,p′-DDT, b173
1,2-Decahydroacenaphthylene, a2
cis-Decalin, d2
trans-Decalin, d3
Decamethylene glycol, d12
Decanealdehyde, d7
1,10-Decanedicarboxylic acid, d805


c387


c388


c395

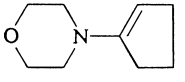


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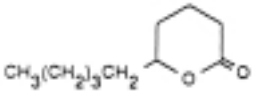
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d13	Decanedioyl dichloride	$ClC(=O)(CH_2)_8COCl$	239.14	2, 719	1.1212_4^{20}	$1,4678^{20}$		220^{75mm}	>110	dec aq, alc
d13a	Decanenitrile	$CH_3(CH_2)_8CN$	153.27	2, 356	0.8295_4^{15}	1.4295^{20}	−15	235–237		misc alc, chl, eth
d14	1-Decanethiol	$CH_3(CH_2)_9SH$	174.35	1^2, 459	0.841	1.4565^{20}	−26	114^{13mm}	98	
d15	Decanoic acid	$CH_3(CH_2)_8COOH$	172.27	2^2, 309	0.8752_4^{50}	1.4288^{40}	32	270	>110	0.015 aq; s alc, bz, chl, CS_2
d16	1-Decanol	$CH_3(CH_2)_9OH$	158.29	1, 425	0.8297_4^{20}	1.4359^{20}	6.9	232	82	i aq; s alc, eth
d17	δ-Decanolactone		170.25	17^5,9, 91	0.954	1.4580^{20}		$120^{0.02mm}$	>110	
d18	2-Decanone	$CH_3(CH_2)_7COCH_3$	156.27	1, 711	0.825	1.4250^{20}	3.5	211	71	
d19	3-Decanone	$CH_3(CH_2)_6COC_2H_5$	156.27	1^1, 367	0.825	1.4241^{20}	−3.8	205	25	
d20	4-Decanone	$CH_3(CH_2)_6C(=O)(CH_2)_2CH_3$	156.27	1, 711	0.824_0^{20}	1.4237^{20}		207	71	i aq; misc alc, eth
d21	Decanoyl chloride	$CH_3(CH_2)_8COCl$	190.71	2, 356	0.919	1.4410^{20}	−34.5	96^{5mm}	106	dec aq. alc; s eth
d22	1-Decene	$H(CH_2)_8CH=CH_2$	140.27	1^3, 858	0.7408^{20}	1.4210^{20}	−66	170.6	47	i aq; misc alc, eth
d23	Decylamine	$H(CH_2)_{10}NH_2$	157.30	4, 199	0.787	1.4360^{20}	12–14	216–218	85	sl s aq; misc alc, bz, eth, acet
d24	Dehydroabeitylamine		285.48	12^4, 3005		1.5460^{20}			>110	
d25	Dehydroacetic acid		168.15	17, 559			111–113	270		at 25°: 22 acet; 18 bz; 5 eth; 3 EtOH; 5 MeOH
d26	Deoxybenzoin	$C_6H_5CH_2COC_6H_5$	196.25	7^2, 368	1.201_4^0		55–56	320	110	i aq; v s alc, eth
d27	Diacetoxydimethyl-silane	$(CH_3)_2Si(OOCCH_3)_2$	176.3		1.054_4^{20}	1.4030^{20}		164–166		
d28	*trans*-1,1-Diacetoxy-2-butene	$(CH_3CO_2)_2CHCH=CHCH_3$	172.18	2, 154	1.057	1.4290^{20}		106^{20mm}	87	
d29	1,1-Diacetoxy-2-propene	$(CH_3CO_2)_2CHCH=CH_2$	158.16	2, 154	1.078	1.4190^{20}		184	78	
d30	Diallylamine	$(H_2C=CHCH_2)_2NH$	97.16	4, 208	0.787	1.4405^{20}	−88	112	15	
d31	Diallyl ether	$(H_2C=CHCH_2)_2O$	98.15	1, 438	0.805_0^{18}	1.4160^{20}		94–95	−6 (OC)	i aq; misc alc, eth
d32	Diallyl maleate	$H_2C=CHCH_2O_2CCH=CH-CO_2CH_2CH=CH_2$	196.20	2^3, 1926	1.073	1.4702^{20}	−47	116^{4mm}	>110	
d33	Diallyl 1,2-phthalate	$C_6H_4(CO_2CH_2CH=CH_2)_2$	246.27	9^3, 4120	1.121	1.5187^{20}		167^{5mm}	>110	
d34	Diallyl sulfide	$(H_2C=CHCH_2)_2S$	114.21	1, 440	0.8877_4^{27}	1.4889^{20}	−85	138	46	sl s aq; misc alc, eth
d35	(+)-*N*,*N*-Diallyl-tartardiamide	$[-CH(OH)CONHCH_2-CH=CH_2]_2$	228.25	4, 218			186–188			

d36	1,2-Diaminoanthraquinone		238.25	14[1], 459			289–291			sl s alc, eth
d37	1,4-Diaminoanthraquinone		238.25	14, 197			265–269			sl s aq, alc; v s bz
d38	1,5-Diaminoanthraquinone		238.25	14, 203			308 dec			
d39	2,6-Diaminoanthraquinone		238.25	14, 215			>325			sl s hot aq, pyr
d40	3,5-Diaminobenzoic acid	$(H_2N)_2C_6H_3COOH$	152.15	14, 453			228	$-H_2O$, 110		sl s aq; s alc, eth

Decyl alcohol, d16
Decyl bromide, b315
Decyl chloride, c94
Decylic acid, d15
Decyl iodide, i29
Decyl mercaptan, d14
Delphinic acid, m184
Dextrose, g8
Diacetone alcohol, h150
1,2-Diacetoxyethane, e137
(Diacetoxyiodo)benzene, i24
Diacetyl, b466
Diacetylmethane, p34
Diallyl, h39
(+)-*N*,*N*′-Diallyltartramide, d35
2,5-Diaminoanisole, m103



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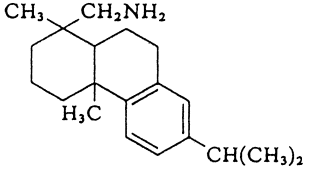

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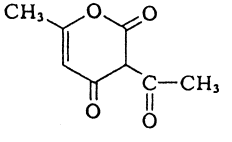

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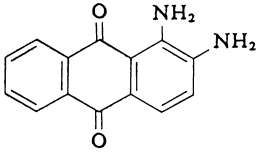

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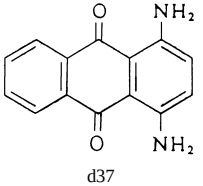

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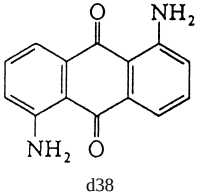

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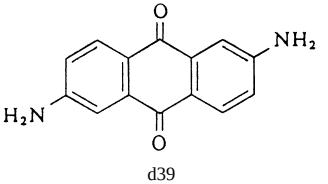


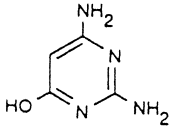
d39

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d41	1,4-Diaminobutane	$H_2N(CH_2)_4NH_2$	88.15	4, 264	0.877	1.4569^{20}	27.3	158–160	51	
d42	4,4′-Diaminodiphenylamine sulfate	$H_2NC_6H_4NHC_6H_4NH_2 \cdot H_2SO_4$	297.33	13, 110			300			s aq
d43	*trans*-1,2-Diaminocyclohexane	$C_6H_{10}(NH_2)_2$	114.19	13^3, 8	0.951	1.2886^{20}	14–15	81^{15mm}	68	
d44	*trans*-1,4-Diaminocyclohexane	$C_6H_{10}(NH_2)_2$	114.19	13^1, 3			69–72	197	71	
d45	*trans*-1,2-Diaminocyclohexane-*N*,*N*,*N*′,*N*′-tetraacetic acid hydrate	$C_6H_{10}[N(CH_2COOH)_2]_2 \cdot H_2O$	364.36	13^3, 10			213–216			v s aq
d46	4,4′-Diaminodiphenylmethane	$H_2NC_6H_4CH_2C_6H_4NH_2$	198.27	13, 238			91–92	398	221	sl s aq; v s alc, bz, eth
d47	3,3′-Diaminodiphenyl sulfone	$H_2NC_6H_4SO_2C_6H_4NH_2$	248.30	13, 426			170–173			i aq; s alc, bz
d48	4,4′-Diaminodiphenyl sulfone	$H_2NC_6H_4SO_2C_6H_4NH_2$	248.30	13, 536			175–176			i aq; s alc, acet, dil HCl
d49	2,4-Diamino-6-hydroxypyrimidine		126.12	24, 469			285 dec			s aq
d50	Diaminomaleonitrile	$NCC(NH_2)=C(NH_2)CN$	108.10	4^2, 949			178–179			
d51	1,8-Diamino-*p*-menthane		170.30	13, 4	0.914	1.4805^{20}	−45	125^{10mm}	93	
d52	3,3′-Diamino-*N*-methyldipropylamine	$CH_3N[(CH_2)_3NH_2]_2$	145.25	4^4, 1279	0.901	1.4725^{20}		112^{6mm}	102	
d53	2,4-Diamino-6-phenyl-1,3,5-triazine		187.21	26^1, 69	1.40_4^{25}		227–228			0.06 aq; s alc, eth, dil HCl; sl s DMF
d54	1,2-Diaminopropane	$CH_3CH(NH_2)CH_2NH_2$	74.13	4, 257	0.878	1.4460^{20}		119–120	33	v s aq
d55	1,3-Diaminopropane	$H_2N(CH_2)_3NH_2$	74.13	4, 261	0.888	1.4570^{20}	−12	140	48	v s aq

d56	1,3-Diamino-2-propanol	$H_2NCH_2CH(OH)CH_2NH_2$	90.13	4, 290			40–45	235	>110	
d58	2,6-Diaminopyridine	$(H_2N)_2C_5H_3N$	109.13	22[1], 647			120–122			s aq, alc
d59	2,4-Diaminotoluene	$(H_2N)_2C_6H_3CH_3$	122.17	13, 124			97–99	283–285		
d60	3,4-Diaminotoluene	$(H_2N)_2C_6H_3CH_3$	122.17	13, 148			91–93	156^{18mm}		
d61	1,4-Diazabicyclo[2.2.2]-octane		112.18	23[3], 484			158–160	174	62	45 aq; 77 EtOH; 51 bz; 13 acet; 26 MeEtKe
d62	1,8-Diazabicyclo[5.4.0]-undec-7-ene		152.24		1.018	1.5219^{20}		$80^{0.6mm}$	>110	
d63	Diazomethane	$CH_2{=}N{=}N$	42.04	23, 25			−145	−23		VERY EXPLOSIVE; s eth, dioxane
d64	1-Diazo-2-naphthol-4-sulfonic acid		272.22	16, 595			160 dec			
d65	1,2,5,6-Dibenz-anthracene		278.33	5[1], 369			266 subl	524		s bz, PE; sl s alc, eth

1,4-Diaminobutane, b455
1,2-Diaminocyclohexane, c354
1,10-Diaminodecane, d9
2,2′-Diaminodiethylamine, d362
1,12-Diaminododecane, d804
1,2-Diaminoethane, e21
1,6-Diaminohexane, h53
1,3-Diamino-2-hydroxypropane, d56
Diaminonaphthalenes, n4, n5
1,2-Diamino-4-nitrobenzene, n66
1,4-Diamino-2-nitrobenzene, n65
1,9-Diaminononane, n91
1,8-Diaminooctane, o24
1,5-Diaminopentane, p30
2,5-Diaminopentanoic acid, o51
1,2-Diaminopropane, p189
1,3-Diaminopropane, p190
4,6-Diamino-4-pyrimidinol, d49
Diaminotoluenes, t167 thru t170
1,3-Diaminourea, c9
Diamylamine, d737
Diamyl ether, d738
Diamyl ketone, u11
Diazirine, d63
1,3-Diazole, i3



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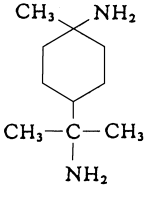

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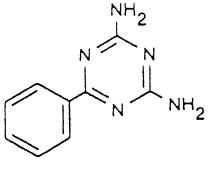

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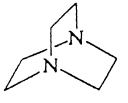

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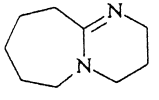

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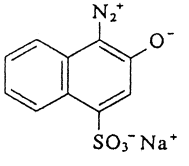

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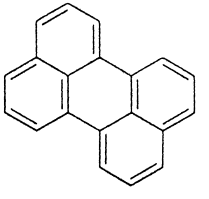
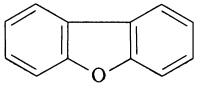

d65

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d66	Dibenzofuran		168.20	17, 70	1.0886_4^{99}	1.6079^{99}	81–83	285		s alc, bz, eth; i aq
d67	Dibenzothiophene		184.26	17, 72			97–100	332–333		s aq; v s alc, bz
d68	Dibenzoylmethane	$C_6H_5COCH_2COC_6H_5$	224.26	7, 769			78–79	220^{18mm}		4.4 alc; s eth, aq NaOH
d69	Dibenzoyl peroxide	$C_6H_5C(=O)OOC(=O)C_6H_5$	242.23	9, 179			103–106	may explode when heated		sl s aq, alc; s bz, chl, eth
d70	(−)-Dibenzoyl-**L**-tartaric acid hydrate	$[(C_6H_5COOCH(COOH)\text{-}]_2 \cdot H_2O$	376.34	9, 170			90–92			
d71	Dibenzylamine	$C_6H_5CH_2NHCH_2C_6H_5$	197.28	12, 1035	1.026	1.5731^{20}	−26	300	143	i aq; s alc, eth
d72	Dibenzyldisulfide	$C_6H_5CH_2SSCH_2C_6H_5$	246.39	6, 465			69	d > 270		s hot alc, bz, eth
d73	Dibenzyl ether	$C_6H_5CH_2OCH_2C_6H_5$	198.27	6, 434	1.0014_4^{20}	1.5168^{20}	2	298	135 (CC)	misc alc, acet, chl, eth
d74	*N,N′*-Dibenzyl-ethylenediamine	$(C_6H_5CH_2NHCH_2\text{-})_2$	240.35	12, 1067	1.024_4^{20}	1.5624^{20}	26	195^{4mm}	>110	v s alc, bz, chl, eth
d75	Dibenzyl malonate	$CH_2[CO_2CH_2C_6H_5]_2$	284.31	6, 436	1.137	1.5447^{20}		$188^{0.2mm}$	>110	
d76	Dibromoacetic acid	$Br_2CHCOOH$	217.86	2, 218			39–41	130^{16mm}	>110	
d77	Dibromoacetonitrile	Br_2CHCN	198.86	2, 219	2.296	1.5393^{20}		69^{24mm}		
d78	2,4′-Dibromoaceto-phenone	$BrC_6H_4C(=O)CH_2Br$	277.96	7, 285			108–110			v s warm alc; s eth
d79	1,4-Dibromobenzene	$C_6H_4Br_2$	235.92	5, 211	0.9641^{100}	1.5743^{100}	87.3	220		1.4 alc; v s eth; s bz
d80	4,4′-Dibromobiphenyl	$BrC_6H_4C_6H_4Br$	312.00	5, 580			167–170	355–360		s bz; sl s hot alc
d81	1,2-Dibromobutane	$CH_3CH_2CH(Br)CH_2Br$	215.93	1, 120	1.789	1.5141^{20}		60^{20mm}	>110	
d82	1,3-Dibromobutane	$CH_3CH(Br)CH_2CH_2Br$	215.93	1, 120	1.800^{20}	1.5085^{20}		175		s chl, eth
d83	1,4-Dibromobutane	$BrCH_2CH_2CH_2CH_2Br$	215.93	1, 120	1.8080_4^{20}	1.5186^{20}	−20	198	110	s chl
d84	*meso*-2,3-Dibromo-butane	$CH_3CH(Br)CH(Br)CH_3$	215.93	1.121	1.767	1.5100^{20}		74^{47mm}	>110	
d85	2,3-Dibromo-1,4-butanediol	$HOCH_2CH(Br)CH(Br)\text{-}CH_2OH$	247.93	1^3, 2176			88–90	$150^{1.5mm}$		
d86	1,4-Dibromo-2,3-butanediol	$BrCH_2C(=O)C(=O)CH_2Br$	243.89	1, 774			117–119			
d87	*trans*-2,3-Dibromo-2-butene-1,4-diol	$HOCH_2C(Br)=C(Br)CH_2OH$	245.91	1^1, 260			112–114			

d88	Dibromochloro-methane	$HCClBr_2$	208.29	1, 67	2,451	1.5465^{20}	−22	120^{748mm}	none	misc alc, bz, eth
d89	*trans*-1,2-Dibromo-cyclohexane	$C_6H_{10}Br_2$	241.96	5, 24	1.784	1.5515^{20}		146^{10mm}	>110	
d90	1,2-Dibromo-2-chloro-1,1,2-trifluoroethane	$FCCl(Br)C(Br)F_2$	276.5		2.2478^{20}	1.4275^{20}		93–94	none	
d91	1,10-Dibromodecane	$Br(CH_2)_{10}Br$	300.09	1[1], 64	1.335^{30}	1.4912^{20}	27	160^{15mm}	>110	sl s alc; s eth
d92	1,2-Dibromo-1,1-difluoroethane	$CH_2BrC(Br)F_2$	223.87	1, 92	2.2238^{20}	1.4456^{20}	−61.3	92.4	none	i aq
d93	Dibromodifluoro-methane	Br_2CF_2	209.81	1[1], 16	2.288^{15}_4	1.4016^{20}	−110	25	none	0.1 aq; misc alc, bz, chl, eth
d94	1,2-Dibromo-3,3-dimethylbutane	$(CH_3)_3CCH(Br)CH_2Br$	243.98	1, 151	1.610	1.5053^{20}		73^{3mm}	83	
d95	1,3-Dibromo-5,5-dimethylhydantoin		185.93				197 dec			
d96	1,1-Dibromoethane	CH_3CHBr_2	187.86	1, 90	2.055^{20}_4	1.5379^{20}		113	none	i aq; v s alc, eth
d97	1,2-Dibromoethane	$BrCH_2CH_2Br$	187.86	1, 90	2.1802^{20}_4	1.5387^{20}	10.0	131.7	none	0.43 aq; misc alc, eth
d98	(1,2-Dibromoethyl)-benzene	$C_6H_5CH(Br)CH_2Br$	263.97	5, 356			70–74	140^{15mm}		
d99	*cis*-1,2-Dibromo-ethylene	$BrCH{=}CHBr$	185.86	1, 190	2.21^{17}_4	1.5431^{18}	−53	112.5	none	s alc, bz, chl, eth
d100	*trans*-1,2-Dibromo-ethylene	$BrCH{=}CHBr$	185.86	1, 190	2.246	1.5505^{18}	−6.5	108	none	
d101	1,2-Dibromoethyltri-chlorosilane	$BrCH_2CH(Br)SiCl_3$	321.3		2.046^{20}_4	1.537^{20}		90^{11mm}		

Dibenzo[*b*,*e*]pyridine, a60
Dibenzoyl, b35
Dibenzyl, d752
Dibenzyl ketone, d767



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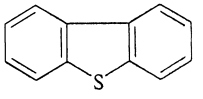
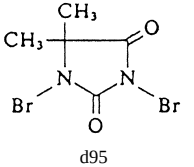


d67



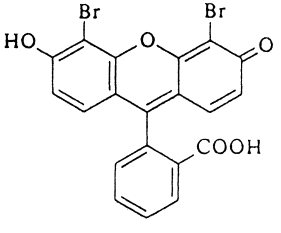
d95

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d102	4′5′-Dibromo-fluorescein		490.12	19, 228			270–273			s hot alc, HOAc
d103	1,4-Dibromo-2-fluoro-benzene	$Br_2C_6H_3F$	253.91	5^4, 684			33–36	216	101	
d104	2,4-Dibromo-1-fluoro-benzene	$Br_2C_6H_3F$	253.91		2.047^{20}	1.5840^{20}		105^{22mm}	92	
d104a	Dibromofluoro-methane	Br_2CHF	191.83				−78	65		
d105	1,2-Dibromohexa-fluoropropane	$CF_3CF(Br)C(Br)F_2$	309.84	1^4, 218	2.169	1.3605^{20}	−95	72^{734mm}	none	
d106	1,6-Dibromohexane	$Br(CH_2)_6Br$	243.98	1, 145	1.586_4^{18}	1.5066^{20}		243	>110	misc eth
d107	2,5-Dibromo-3,4-hexanedione	$CH_3CHBrC(=O)C(=O)$-$CH(Br)CH_3$	271.95	1^3, 3132	1.766	1.5120^{20}		103^{10mm}	>110	
d108	5,7-Dibromo-8-hydroxyquinoline		302.96	21, 97			200–201	subl		s alc, bz; v s eth
d109	2,4-Dibromomesitylene	$1,3,5\text{-}(CH_3)_3\text{-}C_6HBr_2$	278.00	5, 408			61–63	278–279		
d110	Dibromomethane	CH_2Br_2	173.85	1, 67	2.4956_4^{20}	1.5419^{20}	−52.7	96–97	none	1.15 aq; misc alc, bz, acet, chl, eth
d111	2,6-Dibromo-4-methyl-phenol	$Br_2C_6H_2(CH_3)OH$	265.94	6, 406			49–50		>110	
d112	5,7-Dibromo-2-methyl-8-quinolinol		316.99	21^3, 1240			126–130			
d113	1,6-Dibromo-2-naphthol	$Br_2C_{10}H_5OH$	301.98	6, 652			105–107			
d114	2,6-Dibromo-4-nitro-aniline	$Br_2C_6H_2(NO_2)NH_2$	295.93	12, 743			206–208			sl s aq; s HOAc
d115	2,5-Dibromonitro-benzene	$Br_2C_6H_3NO_2$	280.91	5, 250	2.374		82–84			s bz, hot alc
d116	1,8-Dibromooctane	$Br(CH_2)_8Br$	272.03	1, 160	1.477	1.4981^{20}	15–16	272	>110	
d117	1,4-Dibromopentane	$CH_3CH(Br)CH_2CH_2CH_2Br$	229.95	1, 131	1.687	1.5085^{20}	−34	99^{25mm}	>110	
d118	1,5-Dibromopentane	$Br(CH_2)_5Br$	229.95	1, 131	1.6879_4^{15}	1.5092^{20}	−34	110^{15mm}	>110	
d119	2,4-Dibromophenol	$Br_2C_6H_3OH$	251.92	6, 202			40–42	154^{11mm}	>110	

d120	1,2-Dibromopropane	$CH_3CH(Br)CH_2Br$	201.90	1, 109	1.933^{20}	1.5203^{20}	−55.5	142	none	0.2 aq; misc alc, bz, chl, eth
d121	1,3-Dibromopropane	$BrCH_2CH_2CH_2Br$	201.90	1, 110	1.9712^{25}_{4}	1.5233^{20}	−36	166.8	54	0.17 aq; s alc, eth
d122	1,3-Dibromo-2-propanol	$BrCH_2CH(OH)CH_2Br$	217.90	1, 365	2.136	1.5514^{20}		83^{7mm}	46	
d123	2,3-Dibromo-1-propanol	$BrCH_2CH(Br)CH_2OH$	217.90	1, 357	2.120^{20}_{4}	1.5599^{20}		97^{10mm}	>110	sl s aq; misc alc, bz, acet, eth
d124	2,3-Dibromopropene	$BrCH_2C(Br)=CH_2$	199.88	1, 201	1.9336^{20}_{4}	1.5470^{20}		140–143	81	
d125	2,3-Dibromopropionic acid	$BrCH_2CH(Br)COOH$	231.88	2, 258			64–66	160^{20mm}		s aq, alc, bz
d126	2,3-Dibromopropionitrile	$BrCH_2CH(Br)CN$	212.88	2, 259	2.140	1.5450^{20}		173		
d127	2,6-Dibromopyridine	BrC_5H_3N	236.91	20^2, 153			118–119	255		
d128	*meso*-2,3-Dibromosuccinic acid	HOOCCH(Br)CH(Br)COOH	275.89	2, 625			275 subl			v s aq, alc
d129	1,2-Dibromotetrachloroethane	$BrCCl_2CCl_2Br$	325.65	1, 93	2.713		222 dec		none	
d130	1,2-Dibromotetrafluoroethane	$BrCF_2CF_2Br$	259.83		2.149^{25}	1.367^{25}	−110.5	47	none	
d131	2,5-Dibromothiophene	$Br_2C_4H_2S$	241.94	17, 33	2.147^{23}_{23}	1.6289^{20}	−6	211	99	i aq; v s alc, eth
d132	α,α-Dibromotoluene	$C_6H_5CHBr_2$	249.94	5, 308	1.510^{15}	1.6147^{20}		156^{23mm}	>110	i aq; misc alc, eth
d133	1,2-Dibromo-1,1,2-trifluoroethane	$HC(Br)FC(Br)F_2$	241.8	1, 92	2.274^{27}	1.4191^{24}		76.5		
d134	α,α-Dibromo-*o*-xylene	$C_6H_4(CH_2Br)_2$	263.97	5, 366	1.960		92–94			sl s alc, chl, eth

5,7-Dibromo-8-quinolinol, d108



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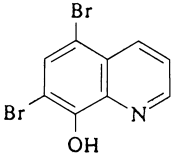

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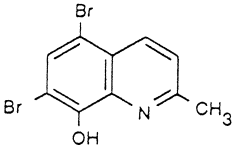


d112

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d135	α,α-Dibromo-*p*-xylene	$C_6H_4(CH_2Br)_2$	263.97	5, 386	1.012^{0}		72–74	261		v s alc, chl; s eth
d136	Dibutoxydibutyltin	$[CH_3(CH_2)_3O]_2Sn[(CH_2)_3CH_3]_2$	379.15		1.110	1.4740^{20}		$138^{0.05mm}$	40	
d137	1,2-Dibutoxyethane	$C_4H_9OCH_2CH_2OC_4H_9$	174.28		0.8374_{20}^{20}	1.4131^{20}	−69.1	203.6	85	0.2 aq; misc alc, acet
d138	Dibutyl adipate	$[-CH_2CH_2CO_2(CH_2)_3CH_3]_2$	258.36	2^2, 575	0.962	1.4360^{20}		305	>110	
d139	Dibutylamine	$(C_4H_9)_2NH$	129.25	4, 157	0.7670^{20}	1.4177^{20}	−62	159.6	47	0.47 aq; s alc, acet, eth EtOAc, PE
d140	Di-*sec*-butylamine	$[C_2H_5CH(CH_3)]_2NH$	129.25	4, 162	0.753	1.4100^{20}		135	20	
d141	*N*,*N*-Dibutylamino-ethanol	$(C_4H_9)_2NCH_2CH_2OH$	173.29	4^3, 682	0.860_{20}^{20}	1.444^{20}	< −70	229–230	91	
d142	*N*,*N*-Dibutylaniline	$C_6H_5N(C_4H_9)_2$	205.34	12^3, 95	0.904^{20}	1.5297^{20}		267–275	>110	i aq, MeOH; s acet, bz, EtOH, EtOAc, eth
d143	Dibutyl decanedioate	$C_4H_9O_2C(CH_2)_8CO_2C_4H_9$	214.45	2, 719	0.9366^{20}	1.4415^{20}	−10	344–345	178	0.004 aq
d144	Di-*tert*-butyl di-carbonate	$(CH_3)_3COC(=O)OC(CH_3)_3$	218.25		0.950	1.4103^{20}	23	$56^{0.5mm}$	37	
d145	2,5-Di-*tert*-butyl-1,4-dihydroxybenzene	$[(CH_3)_3C]_2C_6H_2(OH)_2$	222.33				217–219			
d146	Dibutyl disulfide	$C_4H_9SSC_4H_9$	178.36	1^2, 400	0.9383_4^{20}	1.4920^{20}	−71	231.2	93	i aq; misc alc, eth
d147	Di-*tert*-butyl disulfide	$(CH_3)_3CSSC(CH_3)_3$	178.36		0.935	1.4920		229–233	93	
d148	Dibutyl ether	$C_4H_9OC_4H_9$	130.22	1, 369	0.7689_4^{20}	1.3992^{20}	−95	140	25	0.03 aq; misc alc, eth
d149	2,6-Di-*tert*-butyl-4-(dimethylamino-methyl)phenol	$(CH_3)_2NCH_2C_6H_2$-$[C(CH_3)_3]_2OH$	263.43	13^4, 2014			93–94	172^{30mm}		
d150	*N*,*N*-Dibutylethylene-diamine	$[CH_3(CH_2)_3]_2NCH_2CH_2NH_2$	172.32	4^4, 1182	0.823	1.4430^{20}		117^{24mm}	87	
d151	*N*,*N*-Dibutylformamide	$HC(=O)N(C_4H_9)_2$	157.26		0.864	1.4429^{20}		120^{15mm}	100	
d152	Dibutyl hexanedioate	$[-CH_2CH_2CO_2(CH_2)_3CH_3]_2$	258.36	2^2, 575	0.962	1.4358^{20}		305	>110	
d153	2,5-Di-*tert*-butyl-hydroquinone	$[(CH_3)_3C]_2C_6H_2$-1,4-$(OH)_2$	222.33	6, *3*, 4741			217–219			
d154	Dibutyl maleate	$C_4H_9O_2CCH{=}CHCO_2C_4H_9$	228.29	2^3, 1925	0.9950^{20}	1.4454^{20}	< −80	281	141	0.05 aq
d155	Di-*tert*-butyl malonate	$CH_2CO_2C(CH_3)_3$ | $CO_2C(CH_3)_3$	216.27	2^3, 1621		1.4184^{20}	−6.0	93^{10mm}	88	

d156	2,6-Di-*tert*-butyl-4-methylphenol	$[(CH_3)_3C]_2C_6H_2(CH_3)OH$	220.36	6^3, 2073	1.048_4^{20}	1.4859^{75}	70	265	127	s alc, bz, acet, PE
d157	Dibutyl octanedioate	$[-(CH_2)_3CO_2(CH_2)_3CH_3]_2$	286.41	2^3, 1767	0.948	1.4390^{20}		$176^{4.5mm}$	>110	
d158	Dibutyl oxalate	$C_4H_9O_2CCO_2C_4H_9$	202.25	2, 540	0.986_{20}^{20}	1.4232^{20}	−30.0	239–240	108	misc alc, ketones, PE
d159	Di-*tert*-butyl peroxide	$(CH_3)_3CO{-}OC(CH_3)_3$	146.23	1^3, 1580	0.794^{20}	1.3890^{20}	−40	110	1	misc acet, octane
d160	2,4-Di-*tert*-butylphenol	$[(CH_3)_3C]_2C_6H_3OH$	206.33				56.5	263.5	115	s hot alc; i alk
d161	2,6-Di-*sec*-butylphenol	$[CH_3CH_2CH(CH_3)]_2C_6H_3OH$	206.23		0.918	1.5100^{20}	−42	255–260	127	
d162	2,6-Di-*tert*-butylphenol	$[(CH_3)_3C]_2C_6H_3OH$	206.23	6^3, 2061			35–38	253	118	s hot alc; i alk
d163	3,5-Di-*tert*-butylphenol	$[(CH_3)_3C]_2C_6H_3OH$	206.23				87–89			
d164	Dibutyl phosphite	$(C_4H_9O)_2P(O)H$	194.21	1^1, 187	0.995	1.4239^{20}		119^{11mm}	121	
d165	Dibutyl 1,2-phthalate	C_6H_4 1,2-$[CO_2C_4H_9]_2$	278.35	9^2, 586	1.0465_4^{20}	1.4911^{20}	−35	340	157	0.01 aq; v s alc, bz, acet, eth
d166	*N*,*N*-Dibutyl-1,3-propanediamine	$C_4H_9NH(CH_2)_3NHC_4H_9$	186.34		0.827	1.4463^{20}		205	103	
d167	Dibutyl suberate	$CH_3(CH_2)_3O_2C(CH_2)_6CO_2$-$(CH_2)_3CH_3$	286.41	2^3, 1767	0.948	1.4390^{20}		$175.5^{4.5mm}$	>110	
d168	Dibutyl succinate	$[C_4H_9O_2CCH_2{-}]_2$	230.30	2^2, 551	0.9768_4^{20}	1.4299^{20}	−29.0	274.5		i aq; s alc, eth
d169	Dibutyl sulfate	$C_4H_9OSO_2OC_4H_9$	210.29		1.059_4^{25}	1.4213^{20}		132^{11mm}		
d170	Dibutyl sulfide	$C_4H_9SC_4H_9$	146.30	1, 370	0.8386^{20}	1.4530^{20}	−80	185	76	i aq; v s alc, eth
d171	Di-*tert*-butyl sulfide	$(CH_3)_3CSC(CH_3)_3$	146.30		0.815	1.4506^{20}		151	48	
d172	Dibutyl sulfite	$(C_4H_9O)_2S(=O)$	194.29	1^2, 397	0.9944_4^{22}	1.4310^{20}		108^{15mm}		
d173	Dibutyl sulfone	$(C_4H_9)_2SO_2$	178.29	1, 371			46	295	143	i aq; s alc, eth
d174	Dibutyl **L**-tartrate	$[-CH(OH)CO_2(CH_2)_3CH_3]_2$	262.31	3, 518	1.091	1.4465^{20}	22	175^{5mm}	>110	
d175	*N*,*N*-Dibutyl-2-thiourea	$C_4H_9NC(=S)NHC_4H_9$	188.34				63–65			i aq; s alc; sl s eth
d176	Dibutyltin diacetate	$(CH_3CO_2)_2Sn(C_4H_9)_2$	351.01		1.320	1.4700^{20}		145^{10mm}	>110	
d177	Dibutyltin dichloride	$(C_4H_9)SnCl_2$	303.83				39–41	135^{10mm}	>110	
d178	Dibutyltin dilaurate	$[CH_3(CH_2)_{10}CO_2]_2Sn(C_4H_9)_2$	631.56	Merck: 12, 3089	1.066	1.4683^{20}	22–24		>110	s PE, bz, acet, eth, org esters

Dibutyl adipate, d152
Dibutyl 1,2-benzenedicarboxylate, d165
Dibutyl butanedioate, d168
N,*N*-Dibutyl-1-butanamine, t208
Dibutyl carbitol, b151
Dibutyl cellosolve, d137
Di-*tert*-butylcresol, d156
2,5-Di-*tert*-butylhydroquinone, d145
Dibutyl ketone, n101
Dibutyl sebacate, d143

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

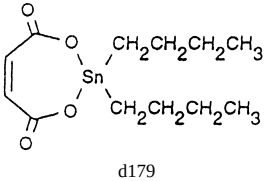
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d179	Dibutyltin maleate		346.98				135–140			
d180	Dibutyltin oxide	$(C_4H_9)_2SnO$	248.92	4[1], 588			> 300			
d181	Dicaprolactone 2-(acryloxy)ethyl ester	$HO(CH_2)_5CO_2(CH_2)_5CO_2$-$CH_2CH_2O_2CCH{=}CH_2$	344.41		1.100	1.4660^{20}			>110	
d182	Dichloroacetic acid	$Cl_2CHCOOH$	128.94	2, 202	1.563_4^{20}	1.4462^{20}	9–11	193–194	>110	misc aq, alc, eth
d183	1,1-Dichloroacetone	$CH_3C(=O)CHCl_2$	126.97	1, 654	1.305_{15}^{18}	1.4455^{20}		120	24	s sl aq; s alc, eth
d184	1,3-Dichloroacetone	$ClCH_2C(=O)CH_2Cl$	126.97	1, 655	1.383		39–41	173	89	
d185	2′,4′-Dichloroaceto-phenone	$Cl_2C_6H_3C(=O)CH_3$	189.04	7, 282		1.5635^{20}	33–34	145^{15mm}	>110	i aq
d186	Dichloroacetyl chloride	$Cl_2CHC(=O)Cl$	147.39	2, 204	1.5315_4^{16}	1.4603^{20}		107–108	none	dec aq, alc; misc eth
d187	2,3-Dichloroaniline	$Cl_2C_6H_3NH_2$	162.02	12, 621		1.5969^{20}	23–24	252	>110	s alc; v s eth
d188	2,4-Dichloroaniline	$Cl_2C_6H_3NH_2$	162.02	12, 621	1.567^{20}		59–62	245		sl s aq; s alc, eth
d189	2,5-Dichloroaniline	$Cl_2C_6H_3NH_2$	162.02	12, 625			49–51	251	>110	s alc, bz, eth
d190	2,6-Dichloroaniline	$Cl_2C_6H_3NH_2$	162.02	12, 626			38–41		>110	
d191	3,4-Dichloroaniline	$Cl_2C_6H_3NH_2$	162.02	12, 626			70–72	272		s alc, eth; sl s bz
d192	3,5-Dichloroaniline	$Cl_2C_6H_3NH_2$	162.02	12, 626			51–53	259^{741mm}	>110	i aq; s alc, eth
d193	1,5-Dichloro-anthraquinone		277.11	7, 787			245–247			sl s alc, bz, acet
d194	2,3-Dichlorobenz-aldehyde	$Cl_2C_6H_3CHO$	175.01	7[3], 878			64–67			
d195	2,4-Dichlorobenz-aldehyde	$Cl_2C_6H_3CHO$	175.01	7, 236			69–73	233		i aq; s alc
d196	2,4-Dichlorobenzamide	$Cl_2C_6H_3CONH_2$	190.03	9[3], 1376			191–194			
d197	2,6-Dichlorobenzamide	$Cl_2C_6H_3CONH_2$	190.03	9[1], 149			196–199			
d198	1,2-Dichlorobenzene	$C_6H_4Cl_2$	147.00	5, 201	1.3059_4^{20}	1.5510^{20}	−17.0	180.4	66	misc alc, bz, eth
d199	1,3-Dichlorobenzene	$C_6H_4Cl_2$	147.00	5, 202	1.2884_4^{20}	1.5460^{20}	−24.8	173.1	72	0.01 aq; s alc, eth
d200	1,4-Dichlorobenzene	$C_6H_4Cl_2$	147.00	5, 203	1.2417^{6}	1.5285^{20}	53	174.1	66	s alc, bz, chl, eth
d201	2,5-Dichlorobenzene-sulfonyl chloride	$Cl_2C_6H_3SO_2Cl$	245.51	11[1], 15			36–37		>110	d hot alc, hot aq
d202	2,4-Dichlorobenzoic acid	$Cl_2C_6H_3COOH$	191.01	9, 342			157–160			s hot aq, alc, bz, chl

d203	2,5-Dichlorobenzoic acid	$Cl_2C_6H_3COOH$	191.01	9, 342			154–157	301		sl s aq; s alc, eth
d204	3,4-Dichlorobenzoic acid	$Cl_2C_6H_3COOH$	191.01	9, 343			207–209			s hot aq, eth; v s alc
d205	4,4′-Dichlorobenzophenone	$(ClC_6H_4)_2C{=}O$	251.11	7, 420			144–146	353		s hot alc, v s chl, eth
d206	2,4-Dichlorobenzotrifluoride	$Cl_2C_6H_3CF_3$	215.00	5^3, 698	1.484	1.4810^{20}		117–118	72	
d207	3,4-Dichlorobenzotrifluoride	$Cl_2C_6H_3CF_3$	215.00	5^3, 698	1.478	1.4750^{20}	−12	173–174	65	
d208	2,4-Dichlorobenzoyl chloride	$Cl_2C_6H_3C(=O)Cl$	209.46	9, 342	1.494	1.5297^{20}	16–18	150^{34mm}	137	dec aq, alc
d209	3,4-Dichlorobenzoyl chloride	$Cl_2C_6H_3C(=O)Cl$	209.46	9, 344			30–33	242	142	dec aq, alc
d210	1,4-Dichlorobutane	$ClCH_2CH_2CH_2CH_2Cl$	127.01	1, 119	1.1598_4^{20}	1.4566^{20}	−38	161–163	40	i aq; s chl
d211	*cis*-1,4-Dichloro-2-butene	$ClCH_2CH{=}CHCH_2Cl$	125.00	1^3, 743	1.188_4^{25}	1.4887^{25}	−48	152	55	i aq; s org solvents
d212	3,4-Dichloro-1-butene	$ClCH_2CH(Cl)CH{=}CH_2$	125.00	1^3, 725	1.150	1.4658^{20}	−61	123	28	
d213	1,4-Dichloro-2-butyne	$ClCH_2C{\equiv}CCH_2Cl$	122.98	1^3, 927	1.258_4^{20}	1.5048^{20}		165–168	160	
d214	Dichloro(2-chloroethyl)methylsilane	$ClCH_2CH_2SiCl_2(CH_3)$	177.53	4^3, 1892	1.261	1.4580^{20}		157^{744mm}	32	
d215	Dichloro(3-chloropropyl)methylsilane	$Cl(CH_2)_3Si(CH_3)Cl_2$	191.56	4^4, 4170	1.227	1.4620^{20}		80^{18mm}	59	
d216	1,10-Dichlorodecane	$Cl(CH_2)_{10}Cl$	211.18	1^3, 522	0.999	1.4605^{20}	15.6	168^{28mm}	>110	
d217	1,1-Dichloro-2,2-diethoxyethane	$Cl_2CHCH(OC_2H_5)_2$	187.07	1, 614	1.138	1.4360^{20}		183–184	60	

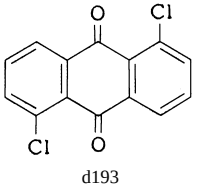
Dichloroacetaldehyde diethyl acetal, d217

2,6-Dichlorobenzyl chloride, t253

2,2′-Dichlorodiethyl ether, b163



d179



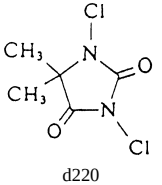
d193

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

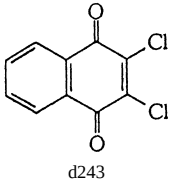
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d218	Dichlorodifluoro-methane	Cl_2CF_2	120.91	1, 61	1.486^{-30}		−158	−29.8		0.01 aq; 9 bz; 5.5 chl; 6 diox; s alc, eth
d219	1,1-Dichloro-3,3-dimethylbutane	$(CH_3)_3CCH_2CHCl_2$	155.07	1^3, 409	1.027	1.4388^{20}	−56	148	36	
d220	1,3-Dichloro-3,5-dimethylhydantoin		197.02	24^2, 158			134–136			
d221	Dichlorodiphenyl-methane	$(C_6H_5)_2CCl_2$	237.13	5, 590	1.235	1.6040^{20}		305	>110	
d222	Dichlorodimethylsilane	$(CH_3)_2SiCl_2$	129.06		1.064_4^{20}	1.4038^{20}	−16	70	−16	
d223	Dichlorodiphenylsilane	$(C_6H_5)_2SiCl_2$	253.20	16, 910	1.222^{20}		308–309	157	dec aq, alc	
d224	1,12-Dichlorododecane	$Cl(CH_2)_{12}Cl$	239.23	1^1, 67			28–30	172^{10mm}	>110	
d225	1,1-Dichloroethane	CH_3CHCl_2	98.96	1, 83	1.1757_4^{20}	1.4164^{20}	−97	57.3	−17	0.51 aq; misc alc
d226	1,2-Dichloroethane	$ClCH_2CH_2Cl$	98.96	1, 84	1.2351_4^{20}	1.4448^{20}	−35.7	83.5	13	0.8 aq; misc alc, chl, eth
d227	1,1-Dichloroethylene	$H_2C{=}CCl_2$	96.94	1, 186	1.2129_4^{20}	1.4247^{20}	−122.6	31.6	−28	0.01 aq; s alc, bz, chl, eth
d228	*cis*-1,2-Dichloro-ethylene	$ClCH{=}CHCl$	96.94	1, 188	1.2838_4^{20}	1.4490^{20}	−80.1	60	2	0.7 aq; s alc, eth
d229	*trans*-1,2-Dichloro-ethylene	$ClCH{=}CHCl$	96.94	1, 188	1.2565^{20}	1.4452^{20}	−49.8	48.7	2	0.6 aq; s alc, eth
d230	2,2′-Dichloroethyl ether	$ClCH_2CH_2OCH_2CH_2Cl$	143.01	1^2, 335	1.2220_{20}^{20}	1.457^{20}		178.5	55	1.1 aq; s alc, bz, eth
d231	2,2-Dichloroethyl methyl ether	$Cl_2CHCH_2OCH_3$	128.99		1.226	1.4375^{20}			33	
d232	Dichloroethylmethyl-silane	$(C_2H_5)Si(CH_3)Cl_2$	143.09		1.063	1.4190^{20}		100	43	
d233	Dichlorofluoro-methane	$FCHCl_2$	102.92	1, 61	1.405^9	1.3724^9	−135	8.9		69 HOAc; 108 diox; s alc, eth; i aq
d234	1,6-Dichlorohexane	$Cl(CH_2)_6Cl$	155.07	1, 144	1.068	1.4568^{20}		87^{15mm}	73	s chl
d235	Dichloromethane	CH_2Cl_2	84.93	1, 60	1.3265^{20}	1.4246^{20}	−95	40	none	1.3 aq; misc alc, eth
d236	Dichloromethane-d_2	CD_2Cl_2	86.95	1^4, 39	1.3621	1.4218^{20}		40	none	

d237	α,α-Dichloromethyl methyl ether	Cl_2CHOCH_3	114.96		1.271	1.4300^{20}		85	42	
d238	Dichloro(methyl)octylsilane	$CH_3(CH_2)_7Si(CH_3)Cl_2$	227.25	4, *4*, 4182	0.973	1.4440^{20}		94^{6mm}	98	
d239	Dichloro(methyl)phenylsilane	$C_6H_5Si(CH_3)Cl_2$	191.13		1.176	1.5190^{20}		205	82	
d240	Dichloro(methyl)silane	$HSi(CH_3)Cl_2$	115.04	4^1, 581	1.105	1.398^{20}	−93	41	−32	
d241	Dichloro(methyl)vinylsilane	$H_2C{=}CHSi(CH_3)Cl_2$	141.07		1.087_4^{20}	1.4300^{20}		92	4	
d242	2,4-Dichloro-1-naphthol	$Cl_2C_{10}H_5OH$	213.06	6, 612			108			
d243	2,3-Dichloro-1,4-naphthoquinone		227.05	7, 729			190–192			sl s alc, bz, eth
d244	2,6-Dichloro-4-nitroaniline	$Cl_2C_6H_2(NO_2)NH_2$	207.02	12, 735			190–192			
d245	2,3-Dichloronitrobenzene	$Cl_2C_6H_3NO_2$	192.00	5, 245	1.721^{14}		61–62	257–258	123	s PE
d246	2,4-Dichloronitrobenzene	$Cl_2C_6H_3NO_2$	192.00	5, 245	1.439^{80}		29–32	258	>110	s hot alc; misc eth
d247	2,5-Dichloronitrobenzene	$Cl_2C_6H_3NO_2$	192.00	5, 245			54–57	266–269	>110	
d248	3,4-Dichloronitrobenzene	$Cl_2C_6H_3NO_2$	192.00	5, 246	1.456^{75}		41–44	256	123	
d249	2,4-Dichloro-6-nitrophenol	$Cl_2C_6H_2(NO_2)OH$	208.00	6, 241			118–120			

5,5′-Dichloro-2,2′-dihydroxydiphenylmethane, m243
1,1-Dichlorodimethyl ether, d237
Dichlorohydrin, d264
Dichloroisopropyl alcohol, d264
2,4-Dichloro-1-methylbenzene, d274
(Dichloromethyl)benzene, d273
4,4′-Dichloro-α-methylbenzhydrol, b169
sym-Dichloromethyl ether, t165a



d220



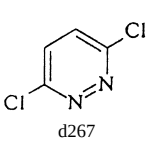
d243

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d250	1,7-Dichloroocta-methyltetrasiloxane	$[Cl(CH_3)_2SiOSi(CH_3)_2\text{-}]_2$	351.53	4^3, 1884	1.011_4^{20}	1.403^{20}	−62	222		
d251	1,5-Dichloropentane	$Cl(CH_2)_5Cl$	141.04	1, 131	1.1058_4^{20}	1.4553^{20}	−72	66^{10mm}	26	i aq; s alc, eth
d252	2,3-Dichlorophenol	$Cl_2C_6H_3OH$	163.00	6^1, 102			58–60	206		s alc, eth
d253	2,4-Dichlorophenol	$Cl_2C_6H_3OH$	163.00	6, 189			42–43	210	113	v s alc, bz, chl, eth
d254	2,5-Dichlorophenol	$Cl_2C_6H_3OH$	163.00	6, 189			56–58	211		v s alc, bz, eth
d255	2,6-Dichlorophenol	$Cl_2C_6H_3OH$	163.00	6, 190			65–68	218–220		v s alc, eth
d256	2,4-Dichlorophenoxy-acetic acid	$Cl_2C_6H_3OCH_2COOH$	221.04				136–140	$160^{0.4mm}$		s alc, bz, chl, eth
d257	4-(2,4-Dichlorophen-oxy)butanoic acid	$Cl_2C_6H_3O(CH_2)_3CO_2H$	249.10	6^3, 708			117–119			46 ppm aq^{25}; s acet, alc, eth; sl s bz
d258	2-(2,4-Dichlorophen-oxy)propanoic acid	$Cl_2C_6H_3OCH(CH_3)CO_2H$	235.07	6, 189			110–112			350 ppm aq^{20}; v s org solvents
d259	3,4-Dichlorophenyl isocyanate	$Cl_2C_6H_3NCO$	188.01	12^3, 1405			42–44	120^{18mm}	>110	
d260	Dichlorophenylphos-phine	$C_6H_5PCl_2$	178.99	16, 763	1.319	1.5980^{20}	−51	222	>112	
d261	4,5-Dichloro-*o*-phthalic acid	$Cl_2C_6H_2(CO_2H)_2$	235.02	9^1, 366			201–203			s aq; v s eth
d262	1,2-Dichloropropane	$CH_3CH(Cl)CH_2Cl$	112.99	1, 105	1.1558^{20}	1.4390^{20}	−100	96	4	0.26 aq; misc alc, bz, chl, eth
d263	1,3-Dichloropropane	$ClCH_2CH_2CH_2Cl$	112.99	1, 105	1.1878_4^{20}	1.4487^{20}	−99.5	120–122	32	v s alc, eth
d264	1,3-Dichloro-2-propanol	$ClCH_2CH(OH)CH_2Cl$	128.99	1, 364	1.198	1.4835^{20}	−4	174.3	85	9.1 aq; misc alc, eth
d265	1,3-Dichloropropene	$ClCH_2CH{=}CHCl$	110.97	1, 199	1.217_4^{20}	1.470^{20}		97–112	25	i aq; s chl, eth
d266	2,3-Dichloro-1-propene	$ClCH_2C(Cl){=}CH_2$	110.97	1, 199	1.204_{25}^{25}	1.4611^{20}		94	10	misc alc; s eth
d267	3,6-Dichloropyridazine		148.98				66–69			
d268	2,6-Dichloropyridine	$Cl_2C_5H_3N$	147.99	20, 231			86–88			
d269	3,5-Dichloropyridine	$Cl_2C_5H_3N$	147.99	20, 231			65–67			
d270	4,7-Dichloroquinoline		198.05	20^3, 3384			84–86	148^{10mm}		
d270a	Dichlorosilane	Cl_2SiH_2	101.01				−122	8.3		

d270b	1,1-Dichlorotetra-fluoroethane	F_3CCFCl_2	170.92		1.455^{25} satd pres-sure	1.3092^{0}	−57	4		
d271	1,2-Dichloro-1,1,2,2-tetrafluoroethane	$ClCF_2CF_2Cl$	170.93	1[3], 152	1.470^{20}_{4} satd pres-sure	1.3092^{20}	−94	3.6		s alc, eth
d272	2,5-Dichlorothiophene	$Cl_2(C_4H_2S)$	153.03	17, 33	1.442	1.5621^{20}	−40.5	162	59	i aq; misc alc, eth
d273	α,α-Dichlorotoluene	$C_6H_5CHCl_2$	161.03	5, 297	1.254	1.5500^{20}	−16/−17	205	92	v s alc, eth
d274	2,4-Dichlorotoluene	$Cl_2C_6H_3CH_3$	161.03	5, 295	1.2460^{20}_{20}	1.5511^{20}	−13	200.5	79	i aq
d275	2,6-Dichlorotoluene	$Cl_2C_6H_3CH_3$	161.03	5, 296	1.254	1.5507^{20}		196–203	82	i aq; s chl
d276	3,4-Dichlorotoluene	$Cl_2C_6H_3CH_3$	161.03	5, 296	1.251^{25}_{25}	1.5472^{20}	−15	209	85	i aq
d277	α,α-Dichloro-*o*-xylene	$C_6H_4(CH_2Cl)_2$	175.06	5, 364			55–57	239–241	107	
d278	α,α-Dichloro-*p*-xylene	$C_6H_4(CH_2Cl)_2$	175.06	5, 384			99–101	254		22.5 acet; 20 bz; 4.5 CCl_4; 11 eth; 18 EtOAc
d279	2,5-Dichloro-*p*-xylene	$Cl_2C_6H_2(CH_3)_2$	175.06	5, 384			71	222		27 acet; 44 bz; 39 eth; 32 EtOAc; 5 MeOH
d280	Dicumyl peroxide	$[C_6H_5C(CH_3)_2]_2O_2$	270.37				39–41		>110	
d281	Dicyandiamide	$H_2NC(=NH)NHCN$	84.08	3, 91	1.400^{25}_{4}		208–211			2.3 aq; 1.3 alc; i bz
d282	1,2-Dicyanobenzene	$C_6H_4(CN)_2$	128.13	9, 815			139–141			v s bz, alc; s hot eth
d283	1,3-Dicyanobenzene	$C_6H_4(CN)_2$	128.13	9, 836			158–160			s alc, bz, chl, eth
d284	1,4-Dicyanobutane	$NC(CH_2)_4CN$	108.14	2, 653	0.951	1.4380^{20}	1–3	295	93	
d285	1,6-Dicyanohexane	$NC(CH_2)_6CN$	136.20	2, 694	0.954	1.4436^{20}	−3.5	185^{15mm}	>110	
d286	2,4-Dicyano-3-methyl-glutaramide	$CH_3CH[CH(CN)CONH_2]_2$	194.19	2[2], 704			159–160			
d287	1,5-Dicyanopentane	$NC(CH_2)_5CN$	122.17	2, 671	0.951	1.4410^{20}		176^{14mm}	>110	

1,1-Dichloro-2-propanone, d184
α,o-Dichlorotoluene, c56
α,p-Dichlorotoluene, c70
1,2-Dicyanoethane, b456



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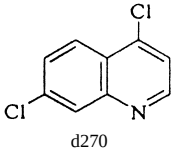


d270

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

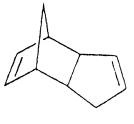
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d288	Dicyclohexyl	$C_6H_{11}C_6H_{11}$	166.31	5, 108	0.864	1.4782^{20}	3–4	227	92	7 MeOH; misc bz, acet, eth
d289	Dicyclohexylamine	$(C_6H_{11})_2NH$	181.32	12, 6	0.910	1.4842^{20}	−2	255.8	96	misc alc, bz, chl, eth
d290	*N,N′*-Dicyclohexylcarbodiimide	$C_6H_{11}N{=}C{=}NC_6H_{11}$	206.33	Merck: 12, 3146			35–36	124^{6mm}	110	
d291	Dicyclohexyl *o*-phthalate	C_6H_4-1,2-$(CO_2C_6H_{11})_2$	330.43	9, 799			64–66			
d292	Dicyclopentadiene		132.21	5, 495	0.930_4^{25}	1.5050^{25}	−1	170	26	s alc, eth
d293	Dicyclopentenyl methacrylate		218.30	6^3, 1942	1.050	1.5080^{20}		137^{13mm}	>110	
d294	Dicyclopropyl ketone	$(C_3H_5)_2C{=}O$	110.16		0.977	1.4670^{20}		160–162	39	
d295	Didodecyl 3,3′-thiodipropionate	$S[CH_2CH_2CO_2(CH_2)_{11}CH_3]_2$	514.86	3^3, 556	0.915		40–42		>110	
d296	Dieldrin		380.92	17^3, 526			176–177			i aq; s common org solvents except PE
d297	Diethanolamine	$HOCH_2CH_2NHCH_2CH_2OH$	105.14	4, 283	1.0881_4^{30}	1.4747^{30}	28.0	269	172	96 aq; 4 bz; 0.8 eth; misc MeOH, acet
d298	2,2-Diethoxyacetophenone	$C_6H_5C(=O)CH(OC_2H_5)_2$	208.26	7^1, 361	1.034	1.4995^{20}		134^{10mm}	>110	
d299	4,4-Diethoxybutylamine	$H_2N(CH_2)_3CH(OC_2H_5)_2$	161.25	4, 319	0.933	1.4275^{20}		196	62	
d300	2,2-Diethoxy-*N,N*-dimethylethylamine	$(C_2H_5O)_2CHCH_2N(CH_3)_2$	161.25	4, 308	0.883	1.4129^{20}		170	45	
d301	Diethoxydimethylsilane	$(C_2H_5O)_2Si(CH_3)_2$	148.28		0.840_4^{20}	1.3811^{20}	−87	114	11	
d302	Diethoxydiphenylsilane	$(C_2H_5O)_2Si(C_6H_5)_2$	272.42	16^2, 608	1.0329_4^{20}	1.5269^{20}		139^{2mm}	>110	
d303	1,1-Diethoxyethane	$CH_3CH(OC_2H_5)_2$	118.18	1, 603	0.8254_4^{20}	1.3819^{20}	−100	102.2	−21	5 aq; misc alc, eth
d304	1,2-Diethoxyethane	$C_2H_5OCH_2CH_2OC_2H_5$	118.18	1, 468	0.842	1.3922^{20}	−74	121.4	27	21 aq
d305	2,2-Diethoxyethanol	$(C_2H_5O)_2CHCH_2OH$	134.18	1, 818	0.888_4^{24}	1.4160^{20}		167	67	s alc, eth
d306	2,2-Diethoxyethylamine	$(C_2H_5O)_2CHCH_2NH_2$	133.19	4, 308	0.916	1.4170		162–163	45	
d307	Diethoxymethane	$(C_2H_5O)_2CH_2$	104.15		0.839	1.3732^{20}		87–88	−5	

d308	3-(Diethoxymethylsilyl)propylamine	$CH_3Si(OC_2H_5)_2(CH_2)_3NH_2$	191.35	4, *4*, 4201	0.916	1.4260^{20}		88^{8mm}	75	
d309	2,5-Diethoxynitrobenzene	$(C_2H_5O)_2C_6H_5NO_2$	211.22	6, 857			48–51	169^{13mm}	>110	
d310	Diethoxymethylvinylsilane	$(C_2H_5O)_2Si(CH_3)CH{=}CH_2$	160.29	4^4, 4183	0.858^{20}_4	1.400^{20}		133–134	17	
d311	1,1-Diethoxypropane	$CH_3CH_2CH(OC_2H_5)_2$	132.20	1, 630	0.8232^{20}_4	1.3884^{20}		122.8	7	v s alc, eth
d312	3,3-Diethoxy-1-propene	$(C_2H_5O)_2CHCH{=}CH_2$	130.19	1, 727	0.854	1.4000^{20}		125	4	
d313	2,2-Diethoxytriethylamine	$(C_2H_5O)_2CHCH_2N(C_2H_5)_2$	189.30	4, 309	0.850	1.4189^{20}		194–195	65	
d314	*N*,*N*-Diethylacetamide	$CH_3C(=O)N(C_2H_5)_2$	115.18	4, 110	0.925	1.4401^{20}		182–186	70	
d315	Diethyl 1,3-acetonedicarboxylate	$C_2H_5OOCCH_2C(=O)CH_2CO_2C_2H_5$	202.21	3, 791	1.113	1.4385^{20}		250	86	
d316	Diethyl 2-acetylglutarate	$C_2H_5O_2CCH_2CH_2CH[C(=O)CH_3]CO_2C_2H_5$	230.26	3, 809	1.071	1.4386^{20}		154^{11mm}	>110	
d317	Diethyl acetylsuccinate	$C_2H_5O_2CCH_2CH[C(=O)CH_3]CO_2C_2H_5$	216.23	3, 801	1.081	1.4346^{20}		183^{50mm}	>110	
d318	Diethyl adipate	$C_2H_5O_2C(CH_2)_4CO_2C_2H_5$	202.25	2, 652	1.009	1.4270^{20}	−18	251	110	
d319	Diethyl allylmalonate	$C_2H_5O_2CCH(CH_2CH{=}CH_2)CO_2C_2H_5$	200.23	2, 776	1.015	1.4304^{20}		222–223	71	
d320	Diethylaluminum chloride	$(C_2H_5)_2AlCl$	120.56	4^3, 1972	0.961		−50	126^{50mm}	−18	
d321	Diethylaluminum ethoxide	$(C_2H_5)_2AlOC_2H_5$	130.17	4^3, 1972	0.850		2.5–4.5	109^{10mm}	−18	
d322	Diethylaluminum iodide	$(C_2H_5)_2AlI$	212.01	4^2, 1024	1.609			120^{4mm}	−18	

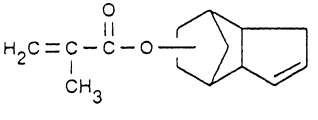
Diethyl acetal, d303

Diethylacetic acid, e100

Diethyl 2-acetylpentanedioate, d316



d292



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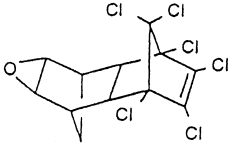


d296

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

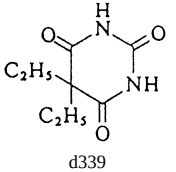
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d323	Diethylamine	$(C_2H_5)_2NH$	73.14	4, 95	0.7074_4^{20}	1.3864^{10}	−50.0	55.5	−23	misc aq, alc
d324	Diethylamine HCl	$(C_2H_5)_2NH \cdot HCl$	109.60	4, 95	1.048_4^{21}		227–230	320–330		s aq, alc, chl; i eth
d325	2-(Diethylamino)-acetonitrile	$(C_2H_5)_2NCH_2CN$	112.18	4, 350	0.866	1.4260^{20}		170	53	
d326	4-(Diethylamino)-benzaldehyde	$(C_2H_5)_2NC_6H_4CHO$	177.25	14^2, 25			39–41	174^{7mm}	>110	
d327	2-Diethylaminoethanol	$(C_2H_5)_2NCH_2CH_2OH$	117.19	4, 282	0.8800^{25}	1.4389^{20}	−70	163	48	s aq, alc, bz, eth
d328	2-Diethylaminoethyl-chloride HCl	$ClCH_2CH_2N(C_2H_5)_2 \cdot HCl$	172.10	4^2, 618			108–210			
d329	2-(Diethylamino)ethyl methacrylate	$H_2C{=}C(CH_3)CO_2CH_2CH_2$-$N(C_2H_5)_2$	185.27	4^3, 676	0.922	1.4440^{20}		80^{10mm}	76	
d330	3-(Diethylamino)-phenol	$(C_2H_5)_2NC_6H_4OH$	165.24	13, 408			65–69	170^{15mm}		s aq, alc, eth
d331	3-Diethylamino-1,2-propanediol	$(C_2H_5)_2NCH_2CH(OH)$-CH_2OH	147.22	4, 302	0.973_{20}^{20}	1.4602^{20}		233–235	107	s aq, alc, chl, eth
d332	1-Diethylamino-2-propanol	$(C_2H_5)_2NCH_2CH(OH)CH_3$	131.22	4^2, 737	0.889	1.4255^{20}	13.5	59^{13mm}	33	s alc
d333	3-Diethylamino-1-propanol	$(C_2H_5)_2NCH_2CH_2CH_2OH$	131.22	4, 288	0.884	1.4435		83^{15mm}	65	
d334	3-Diethylaminopropyl-amine	$(C_2H_5)_2NCH_2CH_2CH_2NH_2$	130.24		0.826	1.4416^{20}		159	58	
d335	*N*,*N*-Diethylaniline	$C_6H_5N(C_2H_5)_2$	149.24	12, 164	0.9302_4^{25}	1.5394^{25}	−38	216	97	1 aq; sl s alc, eth
d336	2,6-Diethylaniline	$(C_2H_5)_2C_6H_3NH_2$	149.24		0.906	1.5452^{20}	3	243	123	
d337	Diethyl azelate	$C_2H_5O_2C(CH_2)_7CO_2C_2H_5$	244.33	2, 709	0.973	1.4350^{20}	−16	172^{18mm}	>110	
d338	Diethyl azodi-carboxylate	$C_2H_5O_2CN{=}NCO_2C_2H_5$	174.16	3, 123	1.106	1.4280^{20}		106^{13mm}	>110	
d339	5,5-Diethylbarbituric acid		184.19	24^2, 279	1.220		188–192			0.7 aq; 7 alc; 1.3 chl; 3.2 eth; s acet, HOAc
d340	Diethyl benzalmalonate	$C_6H_5CH{=}C(CO_2C_2H_5)_2$	248.28	9, 892	1.107	1.5365^{20}		215^{30mm}	>110	
d340a	1,2-Diethylbenzene	$C_6H_4(C_2H_5)_2$	134.22	5, 426	0.880	1.5020^{20}	−31	184	49	
d341	1,3-Diethylbenzene	$C_6H_4(C_2H_5)_2$	134.22	5, 426	0.8640_4^{20}	1.4950^{20}	−83.9	181.1	50	s alc, eth
d342	1,4-Diethylbenzene	$C_6H_4(C_2H_5)_2$	134.22	5, 426	0.8620_4^{20}	1.4940^{20}	−42.8	183.8	56	s alc, eth

d343	Diethyl benzylmalonate	$C_6H_5CH_2CH(CO_2C_2H_5)_2$	250.29	9, 869	1.064	1.4868^{20}		162^{10mm}	>110	
d344	Diethyl benzophosphonate	$C_6H_5CH_2P(O)(OC_2H_5)_2$	228.23	12, 164	1.095	1.4970^{20}		108^{1mm}	>110	
d345	Diethyl bis(hydroxymethyl)malonate	$(HOCH_2)_2C(CO_2C_2H_5)_2$	220.22				49–51		>110	
d346	Diethyl bromomalonate	$BrCH(CO_2C_2H_5)_2$	239.07	2, 594	1.4022_4^{25}	1.4550^{20}	−54	235 dec	>110	i aq; misc alc, eth
d347	Diethyl butylmalonate	$C_4H_9CH(CO_2C_2H_5)_2$	216.28	2[1], 282	0.983	1.4220		235–240	93	v s alc, eth
d348	Diethylcarbamoyl chloride	$(C_2H_5)_2N(O)Cl$	135.59	4, 120	1.070	1.4515^{20}	−32	187–190	75	d hot aq, hot alc
d349	Diethyl carbonate	$(C_2H_5O)_2C{=}O$	118.13	3, 5	0.9764_4^{20}	1.3843^{20}	−43.0	126	25	69 aq; misc alc, bz, eth, esters
d350	Diethyl chlorophosphate	$(C_2H_5O)_2P(O)Cl$	172.55	1, 332	1.194	1.4165^{20}		60^{2mm}	61	
d351	Diethyl chlorothiophosphate	$(C_2H_5O)_2P(S)Cl$	188.61	1[3], 1332	1.200	1.4715^{20}		45^{3mm}	>110	
d352	Diethyl cyanophosphate	$(C_2H_5O)_2P(O)CN$	163.11		1.075	1.4012^{20}		105^{19mm}	80	
d353	*N*,*N*-Diethylcyclohexylamine	$C_6H_{11}N(C_2H_5)_2$	155.29	12, 6	0.850	1.4562^{20}		194–195	57	
d354	Diethyl diethylmalonate	$(C_2H_5)_2C(CO_2C_2H_5)_2$	216.28	2, 686	0.990	1.4230^{20}		228–230	94	
d355	1,3-Diethyl-1,3-diphenylurea	$[C_6H_5N(C_2H_5)]_2C{=}O$	268.36	12, 422			73–75			
d356	Diethyl disulfide	$C_2H_5SSC_2H_5$	122.25	1, 347	0.998_4^{20}	1.5063^{20}	−101.5	154.0	40	sl s aq; misc alc, eth

Diethylaminoacetaldehyde diethyl acetal, d313
3-Diethylaminopropylamine, d400

Diethyl *cis*-2-butanedioate, d377

Diethyl carbitol, b186



d339

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d357	Diethyldithiocarbamic acid, sodium salt	$(C_2H_5)_2NC(=S)S^- Na^+ \cdot 3H_2O$	225.31	4^2, 613			95–99			
d358	Diethyl dithiophosphate	$(C_2H_5O)_2P(S)SH$	186.23	1, 333	1.111	1.5120^{20}		60^{1mm}	82	
d359	*N*,*N*-Diethyldodecanamide	$CH_3(CH_2)_{10}C(=O)N(C_2H_5)_2$	255.45		0.847	1.4545^{20}		166^{2mm}	>110	
d360	Diethyl dodecanedioate	$C_2H_5O_2C(CH_2)_{10}CO_2C_2H_5$	186.41	2^2, 616	0.951	1.4402^{20}	15	193^{14mm}	>110	
d361	Diethylene glycol	$(HOCH_2CH_2)_2O$	106.12	1, 468	1.1197^{15}	1.4460^{20}	−10	246	124	
d362	Diethylenetriamine	$(H_2NCH_2CH_2)NH$	103.17	4, 255	0.9542^{20}_{20}	1.4826^{20}	−35/−39	207	98	misc aq, alc, bz, eth
d363	Diethylenetriaminepentaacetic acid	$[(HO_2CCH_2)_2NCH_2CH_2]_2N(CH_2CO_2H)N(CH_2CO_2H)_2$	393.35	4^4, 2454			219–220			
d364	*N*,*N*-Diethylethanolamine	$HOCH_2CH_2N(C_2H_5)_2$	117.19	4, 282	0.884	1.4410^{20}		161	48	
d365	Diethyl ether	$C_2H_5OC_2H_5$	74.12	1, 314	0.7134^{20}_4	1.3527^{20}	−116.3	34.6	−45	6 aq; misc alc, bz, chl
d366	Diethyl ethoxymethylenemalonate	$(C_2H_5O_2C)_2C=CHOC_2H_5$	216.23	3, 469	1.070	1.4620^{20}		279–281	155	
d367	*N*,*N*-Diethylethylenediamine	$(C_2H_5)_2NCH_2CH_2NH_2$	116.21	4, 251	0.827	1.4360^{20}		145–147	30	
d368	Diethyl ethylmalonate	$C_2H_5CH(CO_2C_2H_5)_2$	188.22	2, 644	1.004^{20}_{20}	1.4158^{20}		77^{5mm}	88	sl s aq; v s alc, eth
d369	*N*,*N*-Diethylformamide	$(C_2H_5)_2NCHO$	101.15	4, 109	0.908	1.4340^{20}		176–177	60	misc aq; v s alc, eth
d370	Diethyl fumarate	$C_2H_5O_2CCH=CHCO_2C_2H_5$	172.18	2, 742	1.052^{20}_4	1.4406^{20}	1–2	218–219	91	
d371	Diethyl glutarate	$C_2H_5O_2CCH_2CH_2CH_2CO_2C_2H_5$	188.22	2, 633	1.022	1.4240^{20}	−23.8	237	96	0.9 aq; v s alc; s eth
d372	2,4-Diethyl-2,6-heptadienal	$H_2C=CHCH_2CH(C_2H_5)CH=C(C_2H_5)CHO$	166.27		0.862	1.4676^{20}		91^{12mm}	86	
d373	Diethyl heptanedioate	$C_2H_5O_2C(CH_2)_5CO_2C_2H_5$	216.28	2, 671	0.9945^{20}	1.4280^{20}	−24	192^{100mm}	>110	i aq; s alc, eth
d374	Di-(2-ethylhexyl)-*o*-phthalate	$C_6H_4[CO_2CH_2CH(C_2H_5)C_4H_9]_2$	390.56	10, 1248	0.981^{25}_{25}	1.4853^{20}	−50	384	207	
d375	Diethyl hydrogen phosphonate	$(C_2H_5O)_2P(O)H$	138.10	1, 330	1.079^{20}_4	1.4076^{20}		51^{2mm}	90	hyd aq; s alc, eth
d376	*N*,*N*-Diethylhydroxylamine	$(C_2H_5)_2NOH$	89.14	4, 536	1.867	1.4195^{20}	−25	125–130	45	
d377	Diethyl maleate	$C_2H_5O_2CCH=CHCO_2C_2H_5$	172.18	2, 751	1.0687^{20}	1.4400^{20}	−8.8	225.3	93	1.4 aq; s alc, eth

d378	Diethyl malonate	$C_2H_5O_2CCH_2CO_2C_2H_5$	160.17	2, 573	1.0550	1.4136^{20}	−49.9	199.3	93	2.7 aq; misc alc, eth
d379	Diethylmalonic acid	$HO_2CC(C_2H_5)_2CO_2H$	160.17	2, 686			127	170–180		v s aq, alc, eth
d380	*N*,*N*-Diethylmethylamine	$(C_2H_5)_2NH_3$	87.17	4, 99	0.720	1.3887^{20}		63–65	−23	
d381	Diethyl methylmalonate	$C_2H_5O_2CCH(CH_3)CO_2C_2H_5$	174.20	2, 629	1.018_4^{20}	1.4130^{20}		198	76	
d382	Diethyl 2-methyl-2′-oxosuccinate	$C_2H_5O_2CCH(CH_3)C(=O)CO_2C_2H_5$	202.21	3, 794	1.073	1.4313^{20}		138^{23mm}	>110	
d383	*N*,*N*-Diethyl-4-nitrosoaniline	$C_6H_4(NO)N(C_2H_5)_2$	178.24	12, 684			82–84			
d384	Diethyl octanedioate	$C_2H_5O_2C(CH_2)_6CO_2C_2H_5$	230.30	2, 693	0.9822_4^{20}	1.4323^{20}	5.9	282	>112	i aq; s alc, eth
d385	Diethyl oxalate	$C_2H_5O_2CCO_2C_2H_5$	146.14	2, 535	1.0785_4^{20}	1.4102^{20}	−40.6	185.4	76	3.6 aq (gradual dec); misc alc, eth
d386	Diethyl oxydiformate	$[C_2H_5OC(=O)]_2O$	162.14	Merck: 12, 8182	1.12_4^{20}	1.3980^{20}		93^{18mm}	69	50 alc; s esters, ketones; s aq
d386a	3,3-diethylpentane	$C(C_2H_5)_4$	128.26		0.7536^{20}	1.4206^{20}	−33	146		
d387	N^1,N^1-Diethyl-1,4-pentanediamine	$CH_3CH(NH_2)(CH_2)_3N(C_2H_5)_2$	158.29	Merck: 12, 6819	0.817	1.4429^{20}		200	68	s aq, alc, eth
d388	N^1,N^1-Diethyl-1,4-phenylenediamine	$(C_2H_5)_2NC_6H_4NH_2$	164.25	13, 75	0.988	1.5710^{20}		116^{5mm}	>110	
d389	Diethyl phenylmalonate	$C_6H_5CH(CO_2C_2H_5)_2$	236.27	9, 854	1.0950_4^{20}	1.4913^{20}	16	170^{14mm}	>110	i aq; s alc
d390	Diethyl phosphite	$(C_2H_5)_2P(O)H$	138.10	1, 330	1.079_4^{20}	1.4079^{20}		51^{2mm}	90	hyd aq; s alc, eth
d391	Diethyl *o*-phthalate	$C_6H_4(CO_2C_2H_5)_2$	222.24	9, 798	1.232_4^{14}	1.5049^{14}	−40	295	160	i aq; misc alc, eth
d392	*N*,*N*-Diethyl-1,3-propanediamine	$(C_2H_5)_2NCH_2CH_2CH_2NH_2$	130.24		0.826	1.4416^{20}		159	58	
d393	2,2-Diethyl-1,3-propanediol	$(C_2H_5)_2C(CH_2OH)_2$	132.20		1.052^{20}	1.4574^{25}	61.3	125^{10mm}		25 aq; v s alc, eth

Diethylene dioxide, d733
Diethylene glycol, b198
Diethylene glycolamine, a164
Diethylene glycol dibutyl ether, b151
Diethylene glycol diethyl ether, b186
Diethylene glycol dimethyl ether, b214
Diethylene glycol monobutyl ether, b495
Diethylene glycol monoethyl ether, e41
Diethylene glycol monoethyl ether acetate, e41a
Diethylene glycol monomethyl ether, m73
Diethyleneimide oxide, m463
N,*N*-Diethylethanamine, t274
Diethyl ethanedioate, d385
N,*N*-Diethylethanolamine, d327
Diethyl ethoxycarbonylmethylphosphonate, t287
Di-2-ethylhexyl phthalate, b193
Diethyl ketone, p43
O,*O*-Diethyl *O*-*p*-nitrophenyl phosphorothioate, p3
Diethyl 3-oxoglutarate, d315
2,3-Diethylpentane, e210a
Diethyl 2-pentenedioate, d371
Diethyl phosphorochloridate, d350
Diethyl phosphorochloridothionate, d351
Diethyl pimelate, d373
Diethyl propanedioate, d378

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d394	Diethyl propyl-malonate	$C_2H_5O_2CCH(C_3H_7)CO_2C_2H_5$	202.25	2, 657	0.987	1.4185^{20}		221–222	91	
d395	Diethyl sebacate	$C_2H_5O_2C(CH_2)_8CO_2C_2H_5$	258.36	2, 717	0.963	1.4360^{20}	1–2	312	>110	0.14 aq; misc alc, eth
d396	Diethyl succinate	$C_2H_5O_2C(CH_2)_2CO_2C_2H_5$	174.20	2, 609	1.040_4^{20}	1.4200^{20}	−21	217.7	100	i aq; misc alc, eth
d397	Diethyl sulfate	$(C_2H_5O)_2SO_2$	154.18	1, 327	1.172_4^{25}	1.4004^{20}	−25	208	78	i aq; misc alc, eth
d398	Diethyl sulfide	$(C_2H_5)_2S$	90.19	1, 344	0.8367_4^{20}	1.4430^{20}	−103.9	92.1	−9	i aq; misc alc, eth
d399	Diethyl sulfite	$(C_2H_5O)_2SO$	138.19	1, 325	1.883	1.450^{20}		158	53	s aq(dec), alc
d400	(+)-Diethyl-**L**-tartrate	$[\text{-}CH(OH)CO_2C_2H_5]_2$	206.19	3, 512	1.205_4^{20}	1.4460^{20}	17	280	93	sl s aq; misc alc, eth
d401	(−)-Diethyl-**D**-tartrate	$[\text{-}CH(OH)CO_2C_2H_5]_2$	206.19	3^1, 181	1.205	1.4460^{20}		162^{19mm}	93	sl s aq; misc alc, eth
d402	*N*,*N*-Diethyl-*m*-toluamide	$CH_3C_6H_4C(=O)N(C_2H_5)_2$	191.27	9^2, 325	0.996_4^{20}	1.5212^{20}		111^{1mm}	>110	i aq; v s alc, bz, eth
d403	*N*,*N*-Diethyl-*m*-toluidine	$CH_3C_6H_4CN(C_2H_5)_2$	163.26	12, 857	0.922	1.5360^{20}		231–232	100	
d404	*N*,*N*-Diethyl-1,1,1-trimethylsilylamine	$(C_2H_5)_2NSi(CH_3)_3$	145.32	4^3, 1861	0.767	1.4110^{20}		125–126	10	
d405	Diethylzinc	$(C_2H_5)_2Zn$	123.49	6, 672	1.2065_4^{20}	1.4983^{20}	−28	118	−23	
d406	1,2-Difluorobenzene	$C_6H_4F_2$	114.09	5^2, 147	1.158	1.4430^{20}	−34	92	2	
d406a	1,4-Difluorobenzene	$C_6H_4F_2$	114.09	5, 199	1.1701^{20}	1.4410^{20}	−13	89	2	
d407	1,1-Difluoroethane	CH_3CHF_2	66.05	1^3, 130	0.909^{21}	1.3011^{-72}	−117	−24.7		0.32 aq
d408	1,1-Difluoroethylene	$CH_2{=}CF_2$	64.04	1, 186			−144	−86		
d409	Difluoromethane	CH_2F_2	52.02	1, 59	2.126 g/L		−136	−51.6		FLAMMABLE GAS
d410	2,4-Difluoronitrobenzene	$F_2C_6H_3NO_2$	159.09	5^1, 129	1.451	1.5110^{20}	9–10	203–204	90	
d411	1,1-Difluorotetrachloroethane	ClF_2CCCl_3	203.83	1, 86	1.649	1.413	41	91	none	sl s alc; v s eth
d412	1,2-Difluorotetrachloroethane	FCl_2CCCl_2F	203.83	1^3, 365	1.6447_4^{25}	1.413^{25}	23.8	203.8		i aq; s alc, eth
d413	Dihexylamine	$(C_6H_{13})_2NH$	185.36	4^1, 384	0.795	1.4320^{20}		192–195	95	s alc, eth
d414	Dihexyl ether	$(C_6H_{13})_2O$	186.34	1^3, 1656	0.7936_4^{20}	1.4204^{20}		226.2	77	i aq; s ethers
d415	9,10-Dihydroanthracene		180.25	5, 641	0.880		108–110	312		i aq; s alc, bz, eth
d416	(+)-Dihydrocarvone		152.24	7^3, 337	0.929^{19}	1.4718^{20}		221–222	81	
d417	Dihydrocoumarin		148.16	17, 315	1.169^{18}	1.5563^{20}	25	272	>110	sl s alc, eth; s chl

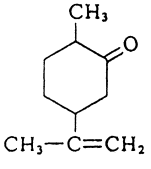
d418	2,5-Dihydro-2,5-dimethoxyfurfurylamine		159.19	18[3], 7426	1.102	1.4600^{20}		96^{12mm}	96	
d419	2,3-Dihydro-2,2-dimethyl-7-benzofuranol		164.21	17[5], *4*, 47	1.101	1.5410^{20}			110	
d420	3,4-Dihydro-2-ethoxy-2*H*-pyran		128.17		0.957	1.4394^{20}		42^{16mm}	24	
d421	2,3-Dihydrofuran		70.09	17[3], 141	0.927	1.4239^{20}		54–55	−24	
d422	3,4-Dihydro-2-methoxy-2*H*-pyran		114.14			1.4425^{20}			16	
d423	3,4-Dihydro-1(2*H*)-naphthalenone		146.19	7, 370	1.099	1.5685^{20}	5–6	116^{6mm}	>110	
d424	3,4-Dihydro-2*H*-pyran		84.12		0.922^{19}_{15}	1.4410^{20}	−70	86	−15	s aq, alc
d425	2′,4′-Dihydroacetophenone	$(HO)_2C_6H_3C(=O)CH_3$	152.15	8, 266	1.180		145–147			s warm alc, HOAc, pyr; i bz, eth

Diethyl pyrocarbonate, d386
Diethyl suberate, d384
Diglycine, i7

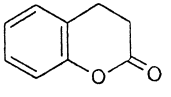
Diglycol, b198
Diglycolic acid, o67
Diglyme, b214

Dihexyl ketone, t264
1,2-Dihydroacenaphthylene, a2
2,5-Dihydroanisole, m67

d415



d416



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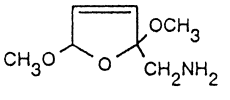
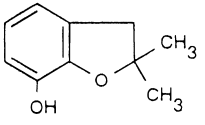


d418



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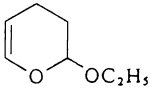
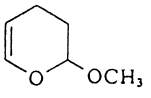
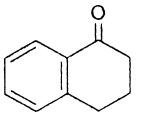


d420

d421



d422



d423

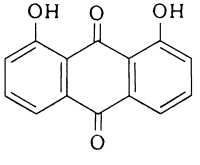
d424

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

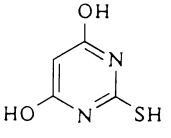
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d426	1,8-Dihydroxyanthra-quinone		240.21	8, 458			193–197	subl		0.005 alc; 0.2 eth; s chl
d427	2,4-Dihydroxybenz-aldehyde	$(HO)_2C_6H_3CHO$	138.12	8, 241			135–136	226^{22mm}		v s aq, alc, chl, eth
d428	1,2-Dihydroxybenzene	$C_6H_4(OH)_2$	110.11	6, 759	1.344^{4}		104–106	245.5	137	43 aq; s alc, bz, chl, eth; v s pyr, alkalis
d429	1,3-Dihydroxybenzene	$C_6H_4(OH)_2$	110.11	6^{2}, 802	1.272^{15}		109–110	276	171	110 aq; 110 alc; v s eth, glyc; sl s chl
d430	1,4-Dihydroxybenzene	$C_6H_4(OH)_2$	110.11	6, 836	1.332^{15}		170–171	285–287		7 aq; v s alc, eth
d431	2,4-Dihydroxybenzoic acid	$(HO)_2C_6H_3CO_2H$	154.12	10, 377			213 rapid heating			s hot aq, alc, eth
d432	2,5-Dihydroxybenzoic acid	$(HO)_2C_6H_3CO_2H$	154.12	10, 384			199–200			0.5 aq; s alc, eth
d433	3,4-Dihydroxybenzoic acid	$(HO)_2C_6H_3CO_2H$	154.12	10, 389	1.54		200–202			2 aq; s alc, eth
d434	3,5-Dihydroxybenzoic acid	$(HO)_2C_6H_3CO_2H$	154.12	10, 404			236 dec			sl s aq; s alc, eth
d435	2,4-Dihydroxybenz-ophenone	$(HO)_2C_6H_3C(=O)C_6H_5$	214.22	8, 312			144–145			v s alc, eth, HOAc
d436	2,2′-Dihydroxybiphenyl	$HOC_6H_4C_6H_4OH$	186.21	6, 989			110	315		s alc, bz, eth; sl s aq
d437	4,6-Dihydroxy-2-mercaptopyrimidine		144.15	24, 476			236			
d438	1,2-Dihydroxy-4-methylbenzene	$(HO)_2C_6H_3CH_3$	124.14	6, 878	1.129_4^{74}	1.5425^{74}	67–69	251		v s aq, alc, eth
d439	1,5-Dihydroxy-naphthalene	$C_{10}H_6(OH)_2$	160.17	6, 980			259 dec			sl s aq; s alc; v s eth
d440	1,6-Dihydroxy-naphthalene	$C_{10}H_6(OH)_2$	160.17	6, 981			138–140			v s alc, eth
d441	2,3-Dihydroxy-naphthalene	$C_{10}H_6(OH)_2$	160.17	6, 982			162–164			v s alc, eth
d442	2,7-Dihydroxy-naphthalene	$C_{10}H_6(OH)_2$	160.17	6, 985			187 dec			sl s aq; v s alc, eth

d443	1,4-Dihydroxy-2-naphthoic acid	$(HO)_2C_{10}H_5CO_2H$	204.19	10, 442			220 dec			
d444	3,5-Dihydroxy-2-naphthoic acid	$(HO)_2C_{10}H_5CO_2H$	204.19	10, 444			277 dec			
d445	1,3-Dihydroxy-2-propanone	$HOCH_2C(=O)CH_2OH$	90.08	1, 846			65–71			v s aq, alc, acet, eth
d446	7-(2,3-Dihydroxypropyl)theophylline		254.25				158			33 aq; 2 alc; 1 chl
d447	3,6-Dihydroxypyridazine		112.09	24, 312			306–308			sl s ahot alc; s hot aq
d448	2,3-Dihydroxypyridine	$(HO)_2C_5H_3N$	111.10	21^{2}, 107			245 dec			
d449	1,4-Diiodobenzene	$C_6H_4I_2$	329.91	5, 227			131–133	285		sl s alc; v s eth
d450	1,4-Diiodobutane	$I(CH_2)_4I$	309.92	1, 123	2.350	1.6212^{20}	6	152^{26mm}	none	
d451	1,2-Diiodoethane	ICH_2CH_2I	281.86	1, 99	2.132^{10}		81–84	200		sl s aq; s alc, eth
d452	Diiodomethane	CH_2I_2	267.84	1, 71	3.325_4^{20}	1.7425^{20}	6	181	>110	0.12 aq; misc alc, bz, eth, PE
d453	1,5-Diiodopentane	$I(CH_2)_5I$	323.94	1, 133	2.177	1.6002^{20}		102^{3mm}	>110	
d454	1,3-Diiodopropane	$I(CH_2)_3I$	295.88	1, 115	2.5755_4^{20}	1.6423^{20}	−13	222	>110	i aq; s chl, eth

10,11-Dihydro-5*H*-dibenz[*b*,*f*]azepine, i9
2,5-Dihydro-2,5-dimethoxyfuran, d501
3,7-Dihydro-3,7-dimethyl-1*H*-pyridine-2,6-dione, t134
Dihydro-2(3*H*)-furanone, b617
2,3-Dihydroindene, i10
Dihydromyrcenol, m313
Dihydroresorcinol, c323
3,7-Dihydro-1,3,7-trimethyl-1*H*-purine-2,6-dione, c1
1,3-Dihydroxyacetone, d445
1,4-Dihydroxybenzene, h86
1,4-Dihydroxycyclohexane, c359
2,2′-Dihydroxydiethylamine, d297
N,*N*-Di(hydroxyethyl)aminoacetic acid, b199
2,2-Dihydroxy-1,3-indandione, i13
2,2-Dihydroxymethyl-1-butanol, e183
1,1-Di(hydroxymethyl)ethylamine, a215
Dihydroxypropane, p191, p192
3,5-Diiodosalicylic acid, h113
Diisobutyl adipate, d459



d426



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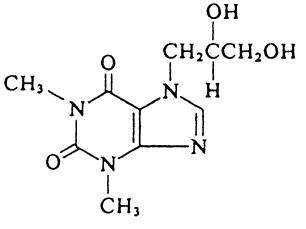
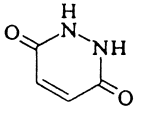


d446



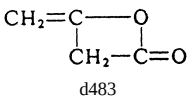
d447

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

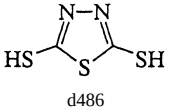
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d455	Diisobutylaluminum chloride	$[(CH_3)_2CHCH_2]_2AlCl$	176.67	4^4, 4403	0.905	1.4506^{20}	−40	152^{10mm}	−18	
d456	Diisobutylaluminum hydride	$[(CH_3)_2CHCH_2]_2AlH$	142.22	4^4, 4400	0.798			118^{1mm}	−18	
d457	Diisobutylamine	$[(CH_3)_2CHCH_2]_2NH$	129.25	4, 166	0.740	1.4081^{20}	−77	137–139	29	s alc, acet, eth, chl
d458	Diisobutyl ether	$[(CH_3)_2CHCH_2]_2O$	130.22		0.761^{15}			122–124	8	i aq; misc alc, eth
d459	Diisobutyl hexanedioate	$[(CH_3)_2CHCH_2O_2CCH_2CH_2^-]_2$	258.36		0.950^{25}_{25}				160	
d460	Diisobutyl *o*-phthalate	$C_6H_4[CO_2CH_2CH(CH_3)_2]_2$	278.35	9^2, 587	1.038^{25}_{25}	1.4900^{20}			174	
d461	1,6-Diisocyanatohexane	$OCN(CH_2)_6NCO$	168.20	4^2, 711	1.040	1.4525^{20}		255	140	
d462	Diisodecyl phenyl phosphite	$(C_{10}H_{21}O)_2P(O)C_6H_5$	438.64		0.940	1.4800^{20}		176^{5mm}		
d463	Diisoheptyl *o*-phthalate	$C_6H_4(CO_2C_7H_{15})_2$			0.990	1.4860^{20}			>110	
d464	Diisononyl *o*-phthalate	$C_6H_4(CO_2C_9H_{19})_2$			0.972	1.4850^{20}			>110	
d465	Diisooctyl nonanedioate	$C_8H_{17}O_2C(CH_2)_7CO_2C_8H_{17}$	412.66		0.905	1.4510^{10}		210^{2mm}	>110	
d466	Diisooctyl *o*-phthalate	$C_6H_4(CO_2C_8H_{17})_2$	390.56		0.983	1.4860^{20}			>110	
d466a	Diisopentyl ether	$[(CH_3)_2CHCH_2CH_2]_2O$	158.28		0.7777^{20}	1.4085^{20}		172.5		
d467	1,3-Diisopropenylbenzene	$C_6H_4[C(CH_3)=CH_2]_2$	158.25		0.925	1.5571^{20}		231	91	
d468	Diisopropylamine	$[(CH_3)_2CH]_2NH$	101.19	4, 154	0.7153^{20}	1.3924^{20}	−61	83.5	−1	11 aq; s alc
d469	2-(Diisopropylamino)ethanol	$[(CH_3)_2CH]_2NCH_2CH_2OH$	145.25	4^1, 430	0.826	1.4417^{20}		187–192	57	
d470	3-Diisopropylamino-1,2-propanediol	$[(CH_3)_2CH]_2NCH_2CH(OH)CH_2OH$	175.27		0.962	1.4583^{20}		131^{10mm}	>110	
d471	2,6-Diisopropylaniline	$[(CH_3)_2CH]_2C_6H_3NH_2$	177.29	12, 168	0.940	1.5332^{20}	−45	257	123	
d472	Diisopropyl azodicarboxylate	$(CH_3)_2CHO_2CNCO_2CH(CH_3)_2$	202.21		1.027	1.4200^{20}		$75^{0.25mm}$	106	
d473	1,3-Diisopropylbenzene	$C_6H_4[CH(CH_3)_2]_2$	162.28	5, 447	0.856^{20}_4	1.4890^{20}	−63	203	76	misc alc, bz, eth, acet
d474	1,4-Diisopropylbenzene	$C_6H_4[CH(CH_3)_2]_2$	162.28	5^2, 339	0.857^{20}_4	1.4889^{20}	−17	204	76	misc alc, bz, acet, eth
d475	Diisopropylcyanamide	$[(CH_3)_2CH]_2NCN$	126.20	4^3, 279	0.839	1.4270^{20}		93^{25mm}	78	

d476	Diisopropyl ether	$[(CH_3)_2CH]_2O$	102.17	1, 362	0.7258_4^{20}	1.3679^{20}	−86.9	68.4	−28	1.2 aq; misc alc, bz, chl, eth
d477	*N*,*N*-Diisopropyl-ethylamine	$[(CH_3)_2CH]_2NC_2H_5$	129.25	4, *4*, 511	0.742	1.4133^{20}	< −50	127	10	
d478	Diisopropyl malonate	$(CH_3)_2CHO_2CCH_2CO_2$-$CH(CH_3)_2$	188.22	2^3, 1620	0.991	1.4120^{20}		95^{12mm}	88	
d479	2,6-Diisopropylphenol	$[(CH_3)_2CH]_2C_6H_3OH$	178.28	6^1, 272	0.962	1.5140^{20}	18	256	110	
d480	Diisopropyl phosphite	$[(CH_3)_2CHO]_2P(O)H$	166.16	1, 363	0.997	1.4070^{20}		$72–75^{20}$	>110	
d481	(+)-Diisopropyl **L**-tartrate	$[-CH(OH)CO_2CH(CH_3)_2]_2$	234.25	3, 517	1.114	1.4387^{20}		152^{12mm}	109	
d482	1,3-Diisopropyl-2-thiourea	$(CH_3)_2CHNHCSNH$-$CH(CH_3)_2$	160.28	4, 155			143–145			
d483	Diketene		84.07	17^3, 4297	1.090	1.4330^{20}		127	34	
d484	*threo*-1,4-Dimercapto-2,3-butanediol	$HSCH_2CH(OH)CH(OH)$-CH_2SH	154.25				42.43			v s aq, alc, chl, eth
d485	2,3-Dimercapto-1-propanol	$HSCH_2CH(SH)CH_2OH$	124.22		1.2385_4^{25}	1.5270^{25}		120^{15mm}	>110	8 aq(dec); s alc, eth
d486	2,5-Dimercapto-1,3,4-thiadiazole		150.24	27, 677			162 dec			
d487	3′4′-Dimethoxy-acetophenone	$(CH_3O)_2C_6H_3COCH_3$	180.20	8^2, 298			49–51	286–288	>110	sl s aq, alc, eth
d488	2,4-Dimethoxyaniline	$(CH_3O)_2C_6H_3NH_2$	153.18	13, 784	1.075		34–37		>110	s alc, bz, eth
d489	2,5-Dimethoxyaniline	$(CH_3O)_2C_6H_3NH_2$	153.18	13, 788			80–82	270		s aq, alc
d490	3,4-Dimethoxyaniline	$(CH_3O)_2C_6H_3NH_2$	153.18	13, 780			88	176^{22mm}		s hot eth
d491	2,5-Dimethoxybenz-aldehyde	$(CH_3O)_2C_6H_3CHO$	166.18	8, 245			49–52	146^{10mm}	>110	
d492	3,4-Dimethoxybenz-aldehyde	$(CH_3O)_2C_6H_3CHO$	166.18	8, 255			42–43	281	>110	v s alc, eth
d493	1,2-Dimethoxybenzene	$C_6H_4(OCH_3)_2$	138.17	6, 771	1.0819^{25}	1.5232^{25}	22.5	206.3	87	sl s aq; s alc, eth

Diisobutylene, t384
Diisobutyl ketone, d616
Diisopropyl ketone, d658
Dimedone, d596



d483



d486

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

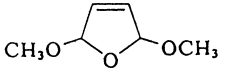
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d494	1,3-Dimethoxybenzene	$C_6H_4(OCH_3)_2$	138.17	6, 813	1.055	1.5240	−55	87^{7mm}	87	s alc, bz, eth
d495	1,4-Dimethoxybenzene	$C_6H_4(OCH_3)_2$	138.17	6, 843	1.036_8^{65}		55–60	213		s alc; v s bz, eth
d496	3,4-Dimethoxybenzoic acid	$(CH_3O)_2C_6H_3CO_2H$	182.18	10^1, 188			180–181			0.05 aq; v s alc, eth
d497	3,5-Dimethoxybenzoic acid	$(CH_3O)_2C_6H_3CO_2H$	182.18	10, 405			182–184			
d498	2,6-Dimethoxybenzoyl chloride	$(CH_3O)_2C_6H_3COCl$	200.62	10^3, 1402			64–66			
d499	3,4-Dimethoxybenzyl alcohol	$(CH_3O)_2C_6H_3CH_2OH$	168.19	5, 1113	1.157	1.5520^{20}		297^{732mm}	>110	
d500	2,2-Dimethoxycyclo-hexanol	$(CH_3O)_2C_6H_9OH$	160.22		1.072	1.4620^{20}		90^{9mm}	40	
d501	2,5-Dimethoxy-2,5-dihydrofuran		130.14		1.073	1.4339^{20}		160–162	47	
d502	Dimethoxydimethyl-silane	$(CH_3O)_2Si(CH_3)_2$	120.23		0.880	1.3690^{20}		81.4	10	
d503	Dimethoxydiphenyl-silane	$(C_6H_5)_2Si(OCH_3)_2$	244.4		1.0771_4^{20}	1.5447^{20}		161^{15mm}		
d504	1,1-Dimethoxyethane	$CH_2CH(OCH_3)_2$	90.12	1, 603	0.8502^{20}	1.3668^{20}	−113	64.5	−17	s aq, alc, chl, eth
d505	1,2-Dimethoxyethane	$CH_3OCH_2CH_2OCH_3$	90.12	1, 467	0.8620_4^{20}	1.3796^{20}	−68	85.2	1	misc aq, alc; s PE
d506	(2,2′-Dimethoxy)-ethylamine	$H_2NCH_2CH(OCH_3)_2$	105.14	4^2, 758	0.965	1.4170^{20}		135^{95mm}	53	
d507	Dimethoxymethane	$CH_2(OCH_3)_2$	76.10	1, 574	0.8601_{20}^{20}	1.3514^{20}	−104.8	42.3	−32	32 aq
d508	1,1-Dimethoxy-2-methylaminoethane	$CH_3NHCH_2CH(OCH_3)_2$	119.16	4^2, 759	0.928	1.4115^{20}		140	29	
d509	Dimethoxymethylvinyl-silane	$CH_3Si(OCH_3)_2CH{=}CH_2$	132.24		0.884	1.3950^{20}		106	3	
d510	Dimethoxymethyl-phenylsilane	$(CH_3O)_2Si(CH_3)C_6H_5$	182.3		0.993_4^{20}	1.469^{20}		199–200		
d511	1,2-Dimethoxy-4-nitrobenzene	$(CH_3O)_2C_6H_3NO_2$	183.16	6, 789	1.1888_4^{133}		95–98	230^{17mm}		v s alc, eth; s chl
d512	2,6-Dimethoxyphenol	$(CH_3O)_2C_6H_3OH$	154.17	6, 1081			53–56	261	>110	s alc, alk; v s eth

d513	3,4-Dimethoxyphenyl-acetic acid	$(CH_3O)_2C_6H_3CO_2H$	196.20	10, 409			96–98			s aq; v s alc, eth
d514	3,4-Dimethoxyphenyl-acetonitrile	$(CH_3O)_2C_6H_3CN$	177.20	10[1], 198			62–63	178^{10mm}		
d515	2,2-Dimethoxy-2-phenylacetophenone	$C_6H_5C(O)C(OCH_3)_2C_6H_5$	256.30				67–70			
d516	1,1-Dimethoxy-2-phenylethane	$C_6H_5CH_2CH(OCH_3)_2$	166.22	7, 293	1.004	1.4950^{20}		221	83	
d517	2-(3,4-Dimethoxy-phenyl)ethylamine	$(CH_3O)_2C_6H_3CH_2CH_2NH_2$	181.24	13, 800	1.074	1.5464^{20}		188^{15mm}	>110	
d518	1,2-Dimethoxypropane	$CH_3CH(OCH_3)CH_2OCH_3$	104.15	1[4], 2471	0.855	1.3835^{20}		96	0	
d519	2,2-Dimethoxypropane	$(CH_3)_2C(OCH_3)_2$	104.15	1, 648	0.847	1.3780^{20}		83	−11	
d520	1,1-Dimethoxy-2-propanone	$CH_3C(O)CH(OCH_3)_2$	118.13	1[1], 395	0.976	1.3978^{20}		143–147	37	
d521	3,3-Dimethoxy-1-propene	$(CH_3O)_2CHCH{=}CH_2$	102.13	1[1], 378	0.862	1.3954^{20}		89–90	−2	
d522	1,2-Dimethoxy-4-propenylbenzene	$CH_3CH{=}CHC_6H_5(OCH_3)_2$	178.23	6, 956	1.055	1.5680^{20}		262–264	>110	
d523	3,3-Dimethoxy-propionitrile	$(CH_3O)_2CHCH_2CN$	115.13	3[4], 521	1.026	1.4130^{20}		92^{30mm}	86	
d524	2,6-Dimethoxypyridine	$(CH_3O)_2C_5H_3N$	139.15		1.053	1.5129^{20}		178–180	61	
d525	2,5-Dimethoxytetra-hydrofuran	$(CH_3O)_2C_4H_6O$	132.16		1.020	1.4180^{20}		145–147	35	
d526	*N*,*N*-Dimethylacet-amide	$CH_3C(O)N(CH_3)_2$	87.12	4, 59	0.9366^{25}	1.4376^{20}	−20	165.5	70	misc aq, alc, bz, eth
d527	2′,6′-Dimethylacet-anilide	$CH_3C(O)NHC_6H_3(CH_3)_2$	163.22	12, 1109			182–184			
d528	Dimethyl 1,3-acetone-dicarboxylate	$[CH_3O_2CCH_2]_2C{=}O$	174.15	3, 790	1.185	1.4434^{20}		150^{25mm}	>110	

3,4-Dimethoxyphenethylamine, d517
1,1-Dimethyoxytrimethylamine, d614

Dimethyl acetal, d504

Dimethylacetic acid, i81



d501

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d529	Dimethyl acetylenedicarboxylate	$CH_3O_2CC{\equiv}CCO_2CH_3$	142.11	2, 803	1.156	1.4470^{20}		98^{19mm}	86	
d530	Dimethyl acetylsuccinate	$CH_3O_2CC_2CH(COCH_3)$-CO_2CH_3	188.18	3^4, 1825	1.160		33	134^{12mm}	>110	
d531	*N*,*N*-Dimethylacrylamide	$H_2C{=}CHC(O)N(CH_3)_2$	99.13	4^3, 130	0.962	1.4730^{20}		81^{20mm}	71	
d532	3,3-Dimethylacrylic acid	$(CH_3)_2C{=}CHCO_2H$	100.12	2, 432			69	195		
d533	Dimethylaluminum chloride	$(CH_3)_2AlCl$	92.51	4^3, 1971	0.996		−21	126–127	−18	
d534	Dimethylamine	$(CH_3)_2NH_2$	45.08	4, 39	0.680^0_4	1.350^{17}	−92.2	6.9	20	v s aq; s alc, eth
d535	Dimethylaminoacetonitrile	$(CH_3)_2NCH_2CN$	84.12	4, 346	0.863	1.4101^{20}		138	36	
d536	4-(Dimethylamino)benzaldehyde	$(CH_3)_2NC_6H_4CHO$	149.19	14, 31			74	176^{17mm}		s alc, chl, eth, HOAc
d537	3-Dimethylaminobenzoic acid	$(CH_3)_2NC_6H_4CO_2H$	165.19	14, 392			148–152			
d538	4-Dimethylaminobenzoic acid	$(CH_3)_2NC_6H_4CO_2H$	165.19	14, 426			241 dec			s alc; sl s eth
d539	2-(Dimethylamino)ethanol	$(CH_3)_2NCH_2CH_2OH$	89.14	4, 276	0.8876^{20}_4	1.4294^{20}		135	40	misc aq, alc, eth
d540	2-[2-(Dimethylamino)ethoxy]ethanol	$(CH_3)_2NCH_2CH_2OCH_2$-CH_2OH	133.19	4^2, 719	0.954	1.4420^{20}		95^{15mm}	92	
d541	2-(Dimethylamino)ethyl acrylate	$H_2C{=}CHCO_2CH_2CH_2$-$N(CH_3)_2$	143.19	4^3, 649	0.943	1.4280^{20}		64^{12mm}	58	
d542	2-(Dimethylamino)ethyl benzoate	$C_6H_5CO_2CH_2CH_2N(CH_3)_2$	193.26		1.014	1.5077^{20}		159^{20mm}	>110	
d543	2-(Dimethylamino)ethyl methacrylate	$H_2C{=}C(CH_3)CO_2CH_2CH_2$-$N(CH_3)_2$	157.22	4^3, 649	0.933	1.4400^{20}		182–192	70	

d544	3-Dimethylamino-phenol	$(CH_3)_2NC_6H_4OH$	137.18	13, 405	1.5895^{25}		82–84	265–268		v s alc, bz, eth, acet
d545	3-Dimethylamino-1,2-propanediol	$(CH_3)_2NCH_2CH(OH)CH_2OH$	119.16	4, 302	1.004	1.4609^{20}		216–217	105	s aq, alc, chl, eth
d546	1-Dimethylamino-2-propanol	$CH_3CH(OH)CH_2N(CH_3)_2$	103.17		0.837	1.4193^{20}		121–127	35	
d547	3-Dimethylamino-1-propanol	$(CH_3)_2NCH_2CH_2OH$	103.17	4[1], 433	0.872	1.4360^{20}		163–164	36	
d548	3-(Dimethylamino)-propionitrile	$(CH_3)_2NCH_2CH_2CN$	98.15	4[3], 1265	0.870	1.4258^{20}	−43	171^{750mm}	62	
d549	3-Dimethylamino-propylamine	$(CH_3)_2N(CH_2)_3NH_2$	102.18	4[3], 554	0.812	1.4350		133	15	
d550	*N*-[3-(Dimethylamino)-propyl]methacryl-amide	$H_2C{=}C(CH_3)CONH(CH_2)_3$-$N(CH_3)_2$	170.26		0.940	1.4790^{20}		134^{2mm}	>110	
d551	4-(Dimethylamino)-pyridine	$(CH_3)_2N(C_5H_4N)$	122.17	22[2], 341			112–114			v s aq, alc, bz, chl
d552	Dimethyl 2-amino-1,4-phthalate	$H_2NC_6H_3(CO_2CH_3)_2$	209.20	14, 559			127–130			
d553	*N*,*N*-Dimethylaniline	$C_6H_5N(CH_3)_2$	121.18	12, 141	0.9559_4^{20}	1.5584^{20}	2.5	194.2	63	v s alc, chl, eth
d554	2,3-Dimethylaniline	$(CH_3)_2C_6H_3NH_2$	121.18	12, 1101	0.9933^{20}	1.5685^{20}	< −15	221–222	97	sl s aq; s alc, eth
d555	2,4-Dimethylaniline	$(CH_3)_2C_6H_3NH_2$	121.18	12, 1111	0.9723^{20}	1.55686^{20}	−14.3	214	90	s alc, bz, eth
d556	2,5-Dimethylaniline	$(CH_3)_2C_6H_3NH_2$	121.18	12, 1135	0.9790_4^{21}	1.5592^{20}	15.5	214	93	sl s aq; s alc, eth
d557	2,6-Dimethylaniline	$(CH_3)_2C_6H_3NH_2$	121.18	12, 1107	0.9842^{20}	1.5601^{20}	11.2	215	96	sl s aq; s alc, eth
d558	3,4-Dimethylaniline	$(CH_3)_2C_6H_3NH_2$	121.18	12, 1103	1.076^{18}		51	228	98	sl s aq; s alc
d559	3,5-Dimethylaniline	$(CH_3)_2C_6H_3NH_2$	121.18	12, 1131	0.9706^{20}	1.5578^{20}	9.8	220.5	93	sl s aq; s alc
d560	Dimethylarsinic acid	$(CH_3)_2As(O)OH$	138.00	4, 610			195–196			v s alc; 200 aq; i eth

cis-2,3-Dimethylacrylic acid, m168
trans-2,3-Dimethylacrylic acid, m169
3,3-Dimethylacrylic acid, m170
Dimethyl adipate, d617
Dimethylaminoacetaldehyde diethyl acetal, d300
Dimethyl 2-amino-1,4-benzenedicarboxylate, d552
Dimethyl 2-aminoterephthalate, d552
N,*N*-Dimethylaminotrimethylsilane, d707
Dimethylanisole, d631, d632
2,4-Dimethyl-3-azapentane, d468

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

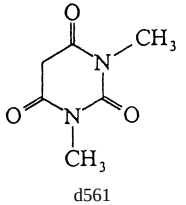
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d561	1,3-Dimethylbarbituric acid		156.14	24, 471			124–126			
d562	*N*,*N*-Dimethylbenzamide	$C_6H_5CON(CH_3)_2$	149.19	9, 201			43–45	133^{15mm}	>110	
d563	3,4-Dimethylbenzoic acid	$(CH_3)_2C_6H_3CO_2H$	150.18	9^2, 353			165–167	subl		s alc, bz
d564	2,5-Dimethylbenzonitrile	$(CH_3)_2C_6H_3CN$	131.18	9, 535	0.957	1.5284^{20}	13–14	223^{730mm}	92	
d565	*N*,*N*-Dimethylbenzylamine	$C_6H_5CH_2N(CH_3)_2$	135.21	12, 1019	0.900	1.5011^{20}	−75	183	54	
d566	2,3-Dimethyl-1,3-butadiene	$H_2C{=}C(CH_3)C(CH_3){=}CH_2$	82.15	1^3, 991	0.7222_4^{25}	1.4362^{25}	−76.0	69.2	−22	
d567	2,2-Dimethylbutane	$CH_3CH_2C(CH_3)_3$	86.18	1, 150	0.6492^{20}	1.3688^{20}	−99.9	49.7	−48	
d568	2,3-Dimethylbutane	$(CH_3)_2CHCH(CH_3)_2$	86.18	1, 151	0.6616^{20}	1.3750^{20}	−128.5	58.0	−29	
d569	2,3-Dimethyl-2,3-butanediol	$(CH_3)_2C(OH)C(OH)(CH_3)_2$	86.18	1, 487			41.1	174.4	77	v s hot aq, alc, eth
d570	2,3-Dimethyl-2-butanol	$(CH_3)_2CHC(CH_3)_2OH$	102.18	1, 413	0.8236_4^{20}	1.4176^{20}	−14	118	29	s aq; misc alc, eth
d570a	3,3-Dimethyl-1-butanol	$(CH_3)_3CCH_2CH_2OH$	102.18	1^3, 1677	0.824^{20}	1.4176^{20}	−60	143	47	
d571	3,3-Dimethyl-2-butanol	$(CH_3)_3CCH(OH)CH_3$	102.18	1, 412	0.8185_4^{20}	1.4151^{20}	5.6	120	28	s alc; misc eth
d572	3,3-Dimethyl-2-butanone	$(CH_3)_3CCOCH_3$	100.16	1, 694	0.7250_{25}^{25}	1.3939^{25}	−52.5	106	23	2.5 aq; s alc, eth
d572a	2,3-Dimethyl-1-butene	$(CH_3)_2CHC(CH_3){=}CH_2$	84.16	1^3, 816	0.680	1.3890^{20}	−157	55.6	−18	
d573	2,3-Dimethyl-2-butene	$(CH_3)_2C{=}C(CH_3)_2$	84.16	1, 218	0.7081_4^{20}	1.4124^{20}	−75	73	−16	s alc, eth
d574	3,3-Dimethyl-1-butene	$(CH_3)_3CCH{=}CH_2$	84.16	1.217	0.6531_4^{20}	1.3762^{20}	−115	41	−28	
d575	*N*,*N*-Dimethylbutylamine	$CH_3(CH_2)_3N(CH_3)_2$	101.19	4, *1*, 371	0.721	1.3980^{20}		93^{750mm}	−3	
d576	2,2-Dimethylbutyric acid	$C_2H_5C(CH_3)_2CO_2H$	116.16	2, 335	0.928	1.4154^{20}		96^{5mm}	79	
d577	3,3-Dimethylbutyric acid	$(CH_3)_3CCH_2CO_2H$	116.16	2, 337	0.9124_4^{20}	1.4100^{20}	6–7	190	88	s alc, eth
d578	Dimethylcadmium	$(CH_3)_2Cd$	142.48		1.9846_4^{17}	1.5488	−4.5	105.5	>150 explodes	dec aq; s PE

d579	Dimethylcarbamyl chloride	$(CH_3)_2NCOCl$	107.54	4, 73	1.168	1.4540^{20}	−33	168	68	
d580	Dimethyl carbonate	$(CH_3O)_2C{=}O$	90.08	3, 4	1.065_4^{17}	1.3682^{20}	0.5	90–91	18	i aq; misc alc, eth
d581	Dimethyl chloromalonate	$ClCH(CO_2CH_3)_2$	166.56	2, 592	1.305	1.4370^{20}		106^{19mm}	106	
d582	Dimethyl chlorothiophosphate	$(CH_3O)_2P(S)Cl$	160.56	1[1], 143	1.322	1.4819^{20}		67^{16mm}	105	
d583	Dimethylcyanamide	$(CH_3)_2NCN$	70.09	4, 74	0.867	1.4100^{20}		161–163	58	
d584	Dimethyl *N*-cyanothioiminocarbonate	$(CH_3S)_2C{=}NCN$	146.23	3, 220			46–50		110	
d584a	1,1-Dimethylcyclohexane	$(CH_3)_2C_6H_{10}$	112.22	5, 35	0.777	1.4280^{20}	−33	120	7	
d585	*cis*-1,2-Dimethylcyclohexane	$(CH_3)_2C_6H_{10}$	112.22	5, 36	0.7963^{20}	1.4335^{20}	−49.9	129.7	16	i aq; s alc, bz
d586	*trans*-1,2-Dimethylcyclohexane	$(CH_3)_2C_6H_{10}$	112.22	5, 36	0.7760^{20}	1.4273^{20}	−90	123.4	11	i aq; s alc, bz
d587	*cis*-1,3-Dimethylcyclohexane	$(CH_3)_2C_6H_{10}$	112.22	5, 36	0.784	1.4230^{20}	−76	120	5	
d587a	*trans*-1,3-Dimethylcyclohexane	$(CH_3)_2C_6H_{10}$	112.22	5[2], 21	0.780	1.4305^{20}	−90	124.5	7	
d588	*cis*-1,4-Dimethylcyclohexane	$(CH_3)_2C_6H_{10}$	112.22	5[2], 22	0.783	1.4297^{20}	−88	125	6	
d589	5,5-Dimethyl-1,3-cyclohexanedione		140.18	7, 559			dec 149			0.4 aq; s alc, bz

Dimethylbenzenes, x4, x5, x6
6,6-Dimethylbicyclo[3.1.1]hept-2-ene-2-ethanol, n106
Dimethyl *cis*-butenedioate, d628

Dimethyl 1-butynedioate, d529
Dimethyl cellosolve, d505
Dimethylchlorosilane, c93

cis-2-Dimethylcrotonic acid, m168
trans-2-Dimethylcrotonic acid, m169



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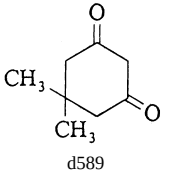


d589

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

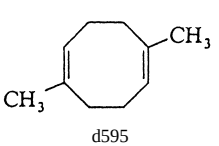
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d590	2,3-Dimethylcyclohexanol	$(CH_3)_2C_6H_9OH$	128.22		0.934	1.4653^{20}			65	
d591	3,5-Dimethylcyclohexanol	$(CH_3)_2C_6H_9OH$	128.22	6, 18	0.892	1.4552	11–12	186	73	
d592	2,6-Dimethylcyclohexanone	$(CH_3)_2C_6H_8(=O)$	126.20	7, 23	0.925	1.4460^{20}		175	51	i aq; s alc, eth
d593	*N*,*N*-Dimethylcyclohexylamine	$C_6H_{11}N(CH_3)_2$	127.23		0.849	1.4535^{20}		159	42	
d594	2,3-Dimethylcyclohexylamine	$(CH_3)_2C_6H_9NH_2$	127.23		0.835	1.4595^{20}		160	51	
d595	1,5-Dimethyl-1,5-cyclooctadiene		136.24		0.867	1.4896^{20}		74^{16mm}	55	
d596	Dimethyl 1,1-cyclopropanedicarboxylate	$C_3H_4(CO_2CH_3)_2$	158.16	9^1, 314	1.147	1.4410^{20}		196–198	95	
d597	Dimethyl decanedioate	$CH_3O_2C(CH_2)_8CO_2CH_3$	230.30	2, 719	0.983^{30}_{20}	1.4335^{28}	23	144^{5mm}	145	i aq; s alc, eth
d598	2,2-Dimethyl-1,3-dioxane-4,6-dione		144.13				94–96			s aq, acet
d599	2,2-Dimethyl-1,3-dioxolane-4-methanol		132.16	19, 65	1.063	1.4340^{20}		188–189	80	misc aq, alc, bz, esters, eth, PE, acetals
d600	Dimethyl disulfide	CH_3SSCH_3	94.20	1, 291	1.0625^{20}	1.5289^{20}	−84.7	109.8	24	i aq; misc alc, eth
d601	Dimethyldithiocarbamic acid, Zn salt	$[(CH_3)_2NCS_2]_2Zn$	305.80	4^3, 149	1.66		250–252			< 0.2 alc, eth; < 0.5 acet, bz; 0.5 naphtha
d602	*N*,*N*-Dimethyldodecylamine	$CH_3(CH_2)_{11}N(CH_3)_2$	213.41	4^3, 409	0.775	1.4375^{20}	−20	112^{3mm}	>110	
d603	Dimethyl ether	$(CH_3)_2O$	46.07	1, 281	0.661^{20}		−141.5	−24.9	−41	35 aq(5 atm); 15 bz; 11.8 acet
d604	*N*,*N*-Dimethylethylamine	$C_2H_5N(CH_3)_2$	73.14	4, 94	0.675	1.3720^{20}	−140	36–38	−36	
d605	*N*,*N*-Dimethylethylenediamine	$C_2H_5NCH_2CH_2NH_2$	88.15	4^2, 690	0.803	1.4260^{20}		106	23	

d606	*N*,*N*-Dimethylformamide	$(CH_3)_2NCHO$	73.10	4, 58	0.9445_4^{25}	1.4305^{20}	−60.4	153.0	57	misc aq, alc, bz, eth
d607	*N*,*N*-Dimethylformamide dimethyl acetal	$(CH_3)_2NCH(OCH_3)_2$	119.16		0.897	1.3972^{20}		103^{720mm}	7	
d608	Dimethyl fumarate	$CH_3O_2CCH{=}CHCO_2CH_3$	144.13	2, 741	1.045^{106}		105	193		sl s alc, eth
d609	2,5-Dimethylfuran	$(CH_3)_2(C_4H_2O)$	96.13	17, 41	0.9000_4^{20}	1.4414^{20}	−62	93	−1	i aq; misc alc, eth
d610	Dimethylglyoxime	$CH_3C(=NOH)$-$C(=NOH)CH_3$	116.12	1, 772			240			s alc, acet, eth, pyr
d611	2,4-Dimethyl-1,6-heptadienal	$H_2C{=}CHCH_2CH(CH_3)$-$CH{=}C(CH_3)CHO$	138.21		0.870	1.4664^{20}		47^{2mm}	64	
d612	2,4-Dimethyl-2,6-heptadien-1-ol	$H_2C{=}CHCH_2CH(CH_3)$-$CH{=}C(CH_3)CH_2OH$	140.23		1.351	1.4640^{20}		86^{10mm}	78	
d613	2,6-Dimethyl-2,5-heptadien-4-one	$(CH_3)_2C{=}CHC(=O)$-$CH{=}(CH_3)_2$	138.21	1, 751	0.885_4^{20}	1.4968^{21}	28	198–199	79	sl s aq; s alc, eth
d613a	2,2-Dimethylheptane	$(CH_3)_3C(CH_2)_4CH_3$	128.26		0.7105^{20}	1.4016^{20}	−113	132.7		
d614	Dimethyl heptanedioate	$CH_3O_2C(CH_2)_5CO_2CH_3$	188.22	2^1, 281	1.0625_4^{20}	1.4314^{20}	−21	122^{11mm}	>110	s alc
d615	2,6-Dimethyl-4-heptanol	$(CH_3)_2CHCH_2CH(OH)$-$CH_2CH(CH_3)_2$	144.26	1, 425	0.809	1.4236^{20}		178	66	
d616	2,6-Dimethyl-4-heptanone	$[(CH_3)_2CHCH_2]_2C{=}O$	142.24	1, 710	0.806_{20}^{20}	1.4114^{20}	−41.5	169.4	49	0.06 aq; misc alc, bz, chl, eth
d616a	2,4-Dimethylhexane	$C_2H_5CH(CH_3)CH_2CH(CH_3)_2$	114.23	1, 162	0.6962^{25}	1.3929^{25}		109.5	10	
d617	Dimethyl hexanedioate	$CH_3O_2C(CH_2)_4CO_2CH_3$	174.20	1, 652	1.0600_4^{20}	1.4285^{20}	8	112^{10mm}	107	i aq; s alc, eth
d618	2,5-Dimethyl-2,5-hexanediol	$[(CH_3)_2C(OH)CH_2{-}]_2$	146.23	1, 492			86–90	214–215	126	

Dimethyl diphenyl sulfone 4,4′-dicarboxylate, s29
Dimethyleneimine, e148
Dimethylene oxide, e146

N,*N*-Dimethylethanolamine, d539
(1,1-Dimethylethyl)benzene, b523
4-(1,1-Dimethylethyl)-4-methylbenzene, b602

4-(1,1-Dimethylethyl)phenol, b588
Dimethyl glutarate, d656



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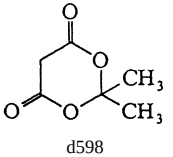

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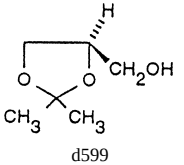


d599

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

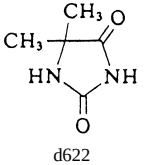
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d619	1,5-Dimethylhexylamine	$(CH_3)_2CH(CH_2)_3CH(NH_2)CH_3$	129.25	Merck: 11, 6678	0.767	1.4209^{20}		154–156	48	
d620	2,5-Dimethyl-3-hexyne-2,5-diol	$(CH_3)_2C(OH)C{\equiv}CC(OH)(CH_3)_2$	142.20	1, 501			94–95	205–206		
d621	3,5-Dimethyl-1-hexyn-3-ol	$(CH_3)_2CHCH_2C(CH_3)(OH)C{\equiv}CH$	126.20	1^2, 507	0.859	1.4335^{20}		151	44	
d622	5,5-Dimethylhydantoin		128.13	24, 289			176–178			v s aq, alc, bz, chl, eth, acet
d623	1,1-Dimethylhydrazine	$(CH_3)_2NNH_2$	60.10	4, 547	0.791_4^{22}	1.4075^{20}	−58	63.9	1	misc aq, alc, eth, PE
d624	1,2-Dimethylhydrazine	$CH_3NHNHCH_3$	60.10	4, 547	0.8274_4^{20}	1.4209^{20}		81	flammable	misc aq, alc, eth, PE
d625	Dimethyl hydrogen phosphonate	$(CH_3O)_2P(O)H$	110.05	1, 285	1.200_4^{20}	1.4009^{20}		170–171	29	s aq(hyd); misc alc, acet, eth
d626	1,2-Dimethylimidazole		96.13	23, 66	1.084		29–30	204	92	
d627	1,3-Dimethyl-2-imidazolidinone		114.15		1.044	1.4720^{20}		108^{17mm}	80	
d628	*N*,*N*-Dimethylisopropylamine	$(CH_3)_2CHN(CH_3)_2$	87.17	4^2, 630	0.715	1.3905^{20}		66	−9	
d629	Dimethyl maleate	$CH_3O_2CCH{=}CHCO_2CH_3$	144.13	2, 751	1.1606^{20}	1.4422^{20}	−19	202	113	8.7 aq
d630	Dimethyl malonate	$CH_3O_2CCH_2CO_2CH_3$	132.12	2, 572	1.154_4^{20}	1.4135^{20}	−62	180–181	90	sl s aq; misc alc, eth
d631	Dimethylmercury	$(CH_3)_2Hg$	230.66	4, 678	3.1874^{20}	1.5452^{20}	−43	92–94	5	i aq; s alc, eth
d632	3,4-Dimethyl-1-methoxybenzene	$(CH_3)_2C_6H_3OCH_3$	136.19	6, 481	0.9744_4^{14}	1.5198^{14}		200		i aq; s alc, bz, eth
d633	3,5-Dimethyl-1-methoxybenzene	$(CH_3)_2C_6H_3OCH_3$	136.19	6, 493	0.9627_4^{15}	1.5107^{15}		193	65	i aq; s alc, bz, eth
d634	Dimethyl methylmalonate	$CH_3CH(CO_2CH_3)_2$	146.14	2, 628	1.098	1.4140^{20}		176–177	76	
d635	Dimethyl methylphosphonate	$(CH_3O)_2P(O)CH_3$	124.08	4^1, 572	1.145	1.4130^{20}		181	68	
d636	Dimethyl methylsuccinate	$CH_3O_2CCH_2CH(CH_3)CO_2CH_3$	160.17	2^3, 1696	1.076	1.4200^{20}		196	83	
d637	2,6-Dimethylmorpholine		115.18		0.9346^{20}	1.4470^{20}	−85	147	48	misc aq, alc, bz

d637a	1,2-Dimethylnaphthalene	$C_{10}H_6(CH_3)_2$	156.23	5[1], 267	1.0179^{20}	1.6166^{20}	0.8	266.5	>110	
d638	1,2-Dimethyl-3-nitrobenzene	$(CH_3)_2C_6H_3NO_2$	151.17	5, 367	1.129	1.5434^{20}	7–9	245	107	i aq; s alc
d639	1,2-Dimethyl-4-nitrobenzene	$(CH_3)_2C_6H_3NO_2$	151.17	5, 368	1.139		29–31	143^{20mm}	>110	i aq; s alc
d640	1,3-Dimethyl-2-nitrobenzene	$(CH_3)_2C_6H_3NO_2$	151.17	5, 378	1.112	1.5220^{20}	14–16	225^{744mm}	87	i aq; s alc
d641	1,3-Dimethyl-4-nitrobenzene	$(CH_3)_2C_6H_3NO_2$	151.17	5, 378	1.117	1.5497^{20}	2	237–239	107	s alc, bz, chl, eth
d642	*N*,*N*-Dimethyl-4-nitrosoaniline	$(CH_3)_2NC_6H_4NO$	150.18	12, 677			86	flammable solid		i aq; s alc, eth
d643	Dimethyl 2-nitro-1,4-phthalate	$O_2NC_6H_3$-1,4-$(CO_2CH_3)_2$	239.18	9, 826			72–75			
d644	*cis*-3,7-Dimethyl-2,6-octadienal		152.24		0.8888^{20}_4	1.4898^{20}		229	101	misc alc, eth, glyc
d645	*trans*-3,7-Dimethyl-2,6-octadienal		152.24		0.8869^{20}_4	1.4869^{20}		229	101	misc alc, eth, glyc
d646	3,7-Dimethyl-1-octanol	$(CH_3)_2CH(CH_2)_3CH(CH_3)$-$CH_2CH_2OH$	158.29	1, 426	0.840	1.4355^{20}		96^{9mm}	95	
d647	3,7-Dimethyl-3-octanol	$(CH_3)_2CH(CH_2)_3$-$C(OH)(CH_3)C_2H_5$	158.29	1, 426	0.826	1.4336^{20}		73^{6mm}	76	

Dimethyl isophthalate, d669
1,4*a*-Dimethyl-7-isopropyl-1,2,3,4,4*a*,9,10,10*a*-octahydro-1-phenanthrenemethylamine, d24

Dimethyl ketone, a26
2,2-Dimethyl-3-methoxyoxirane, m86
6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptane, p176

2,2-Dimethyl-3-methylenebicyclo[2.2.1]heptane, c2
2,2-Dimethyl-3-methylenenorbornane, c2
6,6-Dimethyl-2-methylenenorpinene, p176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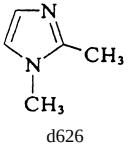
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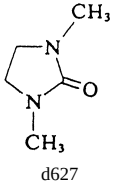
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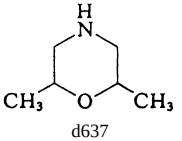
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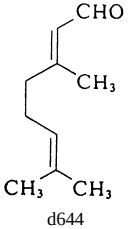
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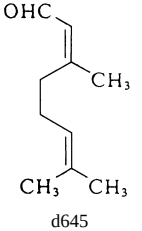

d645

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

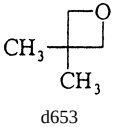
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d648	2,6-Dimethyl-2,4,6-octatriene	$CH_3CH{=}C(CH_3)CH{=}CH\text{-}CH{=}C(CH_3)_2$	136.24	1^{3}, 1050	0.811	1.5429^{20}		75^{14mm}	68	
d649	*N*,*N*-Dimethyloctylamine	$CH_3(CH_2)_7N(CH_3)_2$	157.30	4^{1}, 386	0.765	1.4243^{20}	−57	195	65	
d650	3,6-Dimethyl-4-octyne-3,6-diol	$C_2H_5C(CH_3)(OH)C{\equiv}C\text{-}C(CH_3)(OH)C_2H_5$	170.35	1^{1}, 263			53–55	214^{680mm}	>110	
d651	Dimethyl octanedioate	$CH_3O_2C(CH_2)_6CO_2CH_3$	202.25	2, 693	1.0210_4^{20}	1.4325^{20}	−4.8	268		i aq; s alc
d652	Dimethyl oxalate	$CH_3O_2CCO_2CH_3$	118.09	2, 534	1.148^{54}	1.379^{80}	50–54	163.5	75	6 aq; s alc, eth
d653	3,3-Dimethyloxetane		86.13	17^{2}, 21	0.835	1.3990		81	−9	
d654	2,3-Dimethylpentane	$C_2H_5CH(CH_3)CH(CH_3)_2$	100.21	1^{2}, 120	0.6951_4^{20}	1.3920^{20}		89.8	<−7	i aq; s alc, eth
d655	2,4-Dimethylpentane	$(CH_3)_2CHCH_2CH(CH_3)_2$	100.21	1, 158	0.6727^{20}	$1,3815^{20}$	−120	80.4	−12	
d656	Dimethyl pentanedioate	$CH_3O_2C(CH_2)_3CO_2CH_3$	160.17	2, 633	1.0876^{20}	1.4244^{20}	−42.5	214	102	v s alc, eth
d657	2,4-Dimethyl-3-pentanol	$(CH_3)_2CHCH(OH)CH(CH_3)_2$	116.20	1, 417	0.829_4^{20}	1.4254^{20}		140	37	sl s aq; s alc, eth
d658	2,4-Dimethyl-3-pentanone	$(CH_3)_2CHC(O)CH(CH_3)_2$	114.19	1, 703	0.8062_4^{20}	1.3986^{20}	−69	125	15	
d659	2,3-Dimethylphenol	$(CH_3)_2C_6H_3OH$	122.17	6, 480		1.5420^{20}	72.8	217		v s alc, bz, chl, eth
d660	2,4-Dimethylphenol	$(CH_3)_2C_6H_3OH$	122.17	6, 486	1.0276_4^{14}	1.5420^{14}	24.5	211	>110	v s alc, bz, chl, eth
d661	2,5-Dimethylphenol	$(CH_3)_2C_6H_3OH$	122.17	6, 494	0.965^{80}		74.5	211.5		v s alc, bz, chl, eth
d662	2,6-Dimethylphenol	$(CH_3)_2C_6H_3OH$	122.17	6, 485			45.7	201	73	v s alc, bz, chl, eth
d663	3,4-Dimethylphenol	$(CH_3)_2C_6H_3OH$	122.17	6, 480	0.9830^{20}		60.8	227		v s alc, bz, chl, eth
d664	3,5-Dimethylphenol	$(CH_3)_2C_6H_3OH$	122.17	6, 492	0.9680^{20}		64	222		v s alc, bz, chl, eth
d665	*N*,*N*-Dimethyl-1,4-phenylenediamine	$(CH_3)_2NC_6H_4NH_2$	136.20	13, 72			36	262	90	v s aq; s alc
d666	4,4-Dimethyl-2-phenyl-2-oxazoline		175.23	27^{4}, 1114	1.025	1.5322^{20}	20–24	124^{20mm}	102	
d667	2,2-Dimethyl-3-phenyl-1-propanol	$C_6H_5CH_2C(CH_3)_2CH_2OH$	164.25				35	126^{15mm}	109	
d668	Dimethyl 1,2-phthalate	$C_6H_4(CO_2CH_3)_2$	194.19	9, 797	1.1905^{20}	1.5138^{20}	5.5	283.7	146	0.4 aq; misc alc, chl, eth; i PE
d669	Dimethyl 1,3-phthalate	$C_6H_4(CO_2CH_3)_2$	194.19	9, 834	1.194_4^{20}	1.5168^{20}	67–68	282		i aq
d670	Dimethyl 1,4-phthalate	$C_6H_4(CO_2CH_3)_2$	194.19	9, 843			140–142	288		0.3 hot aq; s hot alc; s eth

d671	1,4-Dimethyl-piperazine		114.19	23, 7	0.844	1.4463^{20}		132^{750mm}	18	
d672	*cis*-2,6-Dimethyl-piperidine		113.20	20, 108	0.840	1.4394^{20}		127	11	
d673	2,2-Dimethylpropane	$(CH_3)_4C$	72.15	Merck: 12, 6545	0.613^{0}	1.3476^{6}	−16.6	9.5	−65	
d674	2,2-Dimethyl-1,3-propanediamine	$H_2NCH_2C(CH_3)_2CH_2NH_2$	102.18	4^3, 595	0.851	1.4566^{20}	31	154	47	
d675	2,2-Dimethyl-1,3-propanediol	$(CH_3)_2C(CH_2OH)_2$	104.15	1, 483	1.11^{25}		127–128	208–210	107	180 aq; 12 bz; 60 acet; v s alc, eth
d676	2,2-Dimethyl-1-propanol	$(CH_3)_3CCH_2OH$	88.15	1, 406	0.812_4^{20}		52.5	113.1	36	3.6 aq; misc alc, eth
d677	2,2-Dimethylpropion-aldehyde	$(CH_3)_3CCHO$	186.25		0.793	1.3794^{20}	6	74^{730mm}	<1	
d678	*N*,*N*-Dimethylpropion-amide	$C_2H_5C(O)N(CH_3)_2$	101.15	4^3, 126	0.920	1.4400^{20}	−45	175	62	
d679	2,2-Dimethylpropionic acid	$(CH_3)_3CCO_2H$	102.13	2, 319	0.905^{50}	1.3931^{37}	35.5	163.8	63	2.5 aq; v s alc, eth
d680	2,2-Dimethylpropionic anhydride	$[(CH_3)_3DD(O)]_2O$	186.25	2, 320	0.918	1.4092^{20}		193	57	
d681	2,2-Dimethylpropionyl chloride	$(CH_3)_3CC(O)Cl$	120.58	2, 320	0.979	1.4120^{20}		105–106	<1	dec aq, alc; v s eth
d682	1,1-Dimethylpropyl-amine	$CH_3CH_2C(CH_3)_2NH_2$	87.17	4, 179	0.731_4^{25}	1.3996^{20}	−105	77	65	misc aq, alc, eth

3,7-Dimethyl-6-octen-1-ol, c275
Dimethylolpropionic acid, b201
Dimethyl 3-oxoglutarate, d325

1,5-Dimethyl-2-phenyl-4-aminopyrazolone, a110
2,3-Dimethyl-1-phenyl-3-pyrazolin-5-one, a299
Dimethyl phosphite, d625

Dimethyl pimelate, d617
Dimethyl propanedioate, d630
1,1-Dimethylpropargylamine, d683



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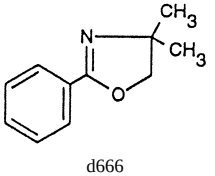

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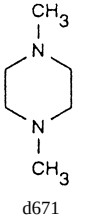

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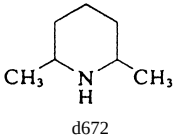


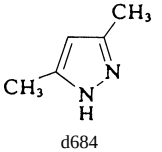
d672

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d683	1,1-Dimethyl-2-propynylamine	$HC{\equiv}CC(CH_3)_2NH_2$	83.13		0.790	1.4235^{20}		79–80	2	
d684	3,5-Dimethylpyrazole		96.13	23, 74			108	218		s aq; v s bz, eth
d685	2,3-Dimethylpyridine	$(CH_3)_2(C_5H_3N)$	107.16	20, 243	0.945	1.5080	−15	163	50	
d686	2,4-Dimethylpyridine	$(CH_3)_2(C_5H_3N)$	107.16	20, 244	0.9309^{20}	1.5010^{20}	< −64	158.3	37	17 aq; v s alc, bz, eth
d687	2,6-Dimethylpyridine	$(CH_3)_2(C_5H_3N)$	107.16	20, 244	0.9226^{20}	1.4956^{20}	−6.0	144	33	43 aq[45]; s alc, eth
d688	3,4-Dimethylpyridine	$(CH_3)_2(C_5H_3N)$	107.16	20, 246	0.954_4^{25}	1.5100^{25}	−12	164	53	sl s aq; s alc, eth
d689	3,5-Dimethylpyridine	$(CH_3)_2(C_5H_3N)$	107.16	20, 246	0.939_4^{25}	1.5033^{25}	−9	170	53	s aq, alc, eth
d690	Dimethyl pyrocarbonate	$O(CO_2CH_3)_2$	134.09	3^4, 17	1.250	1.3933^{20}		46^{5mm}	80	
d691	Dimethyl succinate	$CH_3O_2CCH_2CH_2CO_2CH_3$	146.14	2, 609	1.1198^{20}	1.4190^{20}	19	196.4	85	0.83 aq; 2.9 alc
d692	Dimethylsulfamoyl chloride	$(CH_3)_2NSO_2Cl$	143.59	4, 84	1.337	1.4518^{20}		114^{75mm}	94	
d693	Dimethyl sulfate	$(CH_3O)_2SO_2$	126.13	1, 283	1.3322_4^{20}	1.3874^{20}	−31.8	188 dec	83	2.8 aq(hyd); s acet, bz, dioxane, eth
d694	Dimethyl sulfide	$(CH_3)_2S$	62.13	1, 288	0.8483^{20}	1.4438^{20}	−98.3	37.3	−36	2 aq; s alc, eth
d695	Dimethyl sulfite	$(CH_3O)_2SO$	110.13	1, 282	1.294	1.4083^{20}		126–127	30	
d696	Dimethyl sulfone	$(CH_3)_2SO_2$	94.13	1, 289			109	238	143	v s aq, alc, acet
d697	Dimethyl sulfoxide	$(CH_3)_2SO$	78.13	1, 289	1.101_4^{20}	1.4170^{20}	18.5	189.0	95	s alc, acet, bz, chl
d698	Dimethyl-d_6 sulfoxide	$(CD_3)_2SO$	84.18	1^4, 1279	1.190	1.4758^{20}		55^{5mm}	95	
d699	(+)-Dimethyl L-tartrate	$CH_3O_2CH(OH)CH(OH)CO_2CH_3$	178.14	3, 510	1.328_4^{20}		48–50	163^{23mm}	>110	s aq; 200 alc[15]; v s bz
d700	Dimethyltelluride	$(CH_3)_2Te$	157.68	1, 291			−10	91–92		dec aq; v s alc; i eth
d701	2,5-Dimethyltetrahydrofuran	$(CH_3)_2(C_4H_2O)$	100.16	17, 14	0.833	1.4041		90–92	26	
d702	1,3-Dimethyl-3,4,5,6-tetrahydro-2(1*H*)-pyrimidinone		128.18	24^3, 32	1.060	1.4880^{20}		146^{44mm}	>110	
d703	Dimethyl 3,3′-dithiopropionate	$(CH_3O_2CCH_2CH_2)_2S$	206.26		1.198	1.4740^{20}		148^{18mm}	>110	
d704	*N*,*N*-Dimethylthioformamide	$(CH_3)_2NC(S)H$	89.16	4, 70	1.047	1.5757^{20}		58^{1mm}	99	
d705	*N*,*N*′-Dimethylthiourea	$(CH_3NH)_2C{=}S$	104.18	4, 70			60–62			v s aq, alc, acet

d706	*N*,*N*-Dimethyl-*p*-toluidine	$CH_3C_6H_4N(CH_3)_2$	135.21	12, 902	0.937	1.5458^{20}		211	83	
d707	*N*,*N*-Dimethyltrimethylsilylamine	$(CH_3)_3SiN(CH_3)_2$	117.27		0.732	1.3970^{20}		84	−19	
d708	1,3-Dimethylurea	$(CH_3NH)_2C{=}O$	88.11	4, 65			101–104	268–270		v s aq, alc; i eth
d709	Dimethylzinc	$(CH_3)_2Zn$	95.45	Merck: 12, 3312	0.724		−40	46	−1	misc bz, PE; s eth
d710	2,4-Dinitroaniline	$(O_2N)_2C_6H_3NH_2$	183.12	12, 747	1.615^{14}		176–178			i aq; 0.75 alc
d711	1,3-Dinitrobenzene	$C_6H_4(NO_2)_2$	168.11	5, 258	1.368		89–90	297		0.05 aq; 2.7 alc; v s bz, chl, EtOAc
d712	2,4-Dinitrobenzenesulfenyl chloride	$(O_2N)_2C_6H_3SCl$	234.62	6^2, 316			96			s bz, HOAc; dec alc
d713	3,5-Dinitrobenzoic acid	$(O_2N)_2C_6H_3CO_2H$	212.12	9, 413			205–207			1.9 hot aq; v s alc; sl s bz, eth
d714	3,5-Dinitrobenzoyl chloride	$(O_2N)_2C_6H_3COCl$	230.56	9, 414			69–71	196^{11mm}		dec aq, alc; s eth
d715	2,6-Dinitro-*p*-cresol	$(O_2N)_2C_6H_2(OH)CH_3$	198.13	6, 414			77–79			
d716	4,6-Dinitro-*o*-cresol	$(O_2N)_2C_6H_2(OH)CH_3$	198.13	6, 368			83–87			v s alc, acet, eth, alk
d717	2,4-Dinitrodiphenylamine	$(O_2N)_2C_6H_3NHC_6H_5$	259.22	12, 751			159–161			
d718	2,4-Dinitro-1-fluorobenzene	$FC_6H_3(NO_2)_2$	186.10	5, 262	1.482	1.5690^{20}	27–30	178^{25mm}	>110	s bz, eth, glyc
d719	1,5-Dinitronaphthalene	$C_{10}H_6(NO_2)_2$	218.17	5, 558			216–217	subl		s bz; v s eth; sl s alc

1,3-Dimethyl-2,4,6(1*H*,3*H*,5*H*)pyrimidinetriol, d561
N′-(4,6-Dimethyl-2-pyrimidinyl)sulfanilamide, s22
Dimethyl sebacate, d597
Dimethyl suberate, d651
Dimethyl terephthalate, d670
2,4-Dinitrochlorobenzene, c114
3,4-Dinitrochlorobenzene, c115



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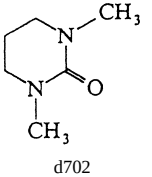

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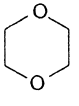
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d720	2,4-Dinitrophenol	$(O_2N)_2C_6H_3OH$	184.11	6, 251	1.683		106–108			s alc, bz; 16 EtOAc; 36 acet; 5 chl; 20 pyr
d721	2,4-Dinitrophenyl-hydrazine	$(O_2N)_2C_6H_3NHNH_2$	198.14	15, 489			*ca.* 200			sl s aq, alc; s acid
d722	3,5-Dinitrosalicylic acid	$(O_2N)_2C_6H_2(OH)CO_2H$	228.12	10, 122			169–172			s aq; v s alc, eth
d723	2,4-Dinitrotoluene	$CH_3C_6H_3(NO_2)_2$	182.14	5, 339	1.321^{71}	1.442	67–70	300 sl d		1.2 alc; 9 eth
d724	2,6-Dinitrotoluene	$CH_3C_6H_3(NO_2)_2$	182.14	5, 341	1.2833^{111}	1.479	64–66			s alc
d725	Dinonyl hexanedioate	$C_9H_{19}O_2C(CH_2)_4CO_2C_9H_{19}$	398.63		0.917^{25}_{25}				218	
d726	Dioctadecyl phosphite	$(C_{18}H_{37}O)_2P(O)H$	586.97				57–59			
d727	Dioctadecyl 3,3′-thiopropionate	$S[CH_2CH_2CO_2(CH_2)_{17}CH_3]_2$	683.18				65–67			
d728	Dioctylamine	$(C_8H_{17})_2NH$	241.46	4, 196	0.799	1.4432^{20}	14–16	298	>110	i aq; v s alc, eth
d729	Dioctyl ether	$(C_8H_{17})_2O$	242.45	1, 419	0.806	1.4318^{20}	−7.6	287	>110	
d730	Dioctyl sulfide	$(C_8H_{17})_2S$	258.51	1, 419	0.842	1.4610^{20}		180^{10mm}	>110	
d731	4,9-Dioxa-1,12-dodecanediamine	$H_2N(CH_2)_3O(CH_2)_4O(CH_2)_3NH_2$	204.32		0.962	1.4609^{20}		136^{4mm}	>110	
d732	1,3-Dioxane		88.11	19, 2	1.032	1.4180^{20}	−45	106	15	
d733	1,4-Dioxane		88.11	19, 3	1.0329^{20}_4	1.4224^{20}	11.8	101.2	12	misc aq, alc, bz, chl, eth, PE
d734	1,3-Dioxolane		74.08	19^2, 2	1.060^{20}_4	1.4000^{20}	−95	78	2	misc aq; s alc, eth
d735	Dipentaerythritol	$(HOCH_2)_3CCH_2OCH_2C(CH_2OH)_3$	254.28				215–218			
d736	Dipentene		136.24	5, 137	0.8402^{21}_4	1.4739^{20}	−95.5	178	45	i aq; misc alc
d737	Dipentylamine	$(C_5H_{11})_2NH$	157.29	4^1, 378	0.777	1.4272		195–202	52	v s alc, eth
d738	Dipentyl ether	$(C_5H_{11})_2O$	158.29	1^1, 193	0.7833^{20}_4	1.4120^{20}	−69.4	190	57	misc alc, eth; s acet
d739	*N*,*N*-Diphenylacetamide	$CH_3CON(C_6H_5)_2$	211.26	12, 247			103	$130^{0.02mm}$		sl s aq; s alc, eth
d740	Diphenylacetic acid	$(C_6H_5)_2CHCO_2H$	212.25	9, 673	1.258^{15}_{15}		148	195^{5mm}		s hot aq, alc, chl, eth
d741	Diphenylacetonitrile	$(C_6H_5)_2CHCN$	193.25	9, 674			71–73	181^{12mm}		
d742	Diphenylacetylene	$C_6H_5C{\equiv}CC_6H_5$	178.23	5, 656	0.990		62.5	300		v s eth, hot alc
d743	Diphenylamine	$(C_6H_5)_2NH$	169.23	12, 174	1.160		53	302	152	45 alc; v s bz, eth

d744	*cis*,*trans*-1,4-Diphenyl-1,3-butadiene	$C_6H_5CH{=}CHCH{=}CHC_6H_5$	206.29	5, 676	0.9974_4^{22}	1.0653^{22}	149.7	350^{720mm}		s alc; sl s eth
d745	Diphenylcarbamoyl chloride	$(C_6H_5)_2NC(O)Cl$	231.68				82–84			
d746	1,5-Diphenylcarbohydrazide	$(C_6H_5NHNH)_2C{=}O$	242.28	15, 292			168–171			s hot alc, acet, HOAc
d747	Diphenyl carbonate	$(C_6H_5O)_2C{=}O$	214.22	6, 158			80–81	301–302		s hot alc, bz, eth
d748	Diphenyl chlorophosphate	$(C_6H_5O)_2P(O)Cl$	268.64	6, 179	1.296	1.5500^{20}		316^{272mm}	>110	
d749	Diphenyl diselenide	$C_6H_5SeSeC_6H_5$	312.13	6, 346	1.557_4^{80}		61–63			s hot alc
d750	Diphenyl disulfide	$C_6H_5SSC_6H_5$	218.34	6, 323	1.353_4^{20}		58–60	310		s alc, bz, eth; i aq
d751	Diphenylenimine		167.21	20, 433	1.10_4^{18}		246	355		0.8 bz; 3 eth; 16 pyr; 11 acet; i aq
d752	1,2-Diphenylethane	$C_6H_5CH_2CH_2C_6H_5$	182.27	5, 598	0.995_4^{20}	1.5338	52.5	284	>110	s alc; v s chl, eth
d753	Diphenyl ether	$C_6H_5OC_6H_5$	170.21	6, 146	1.0661_4^{30}	1.5763^{30}	26.9	258	112	s alc, bz, eth, HOAc
d754	*N*,*N*′-Diphenylformamidine	$C_6H_5N{=}CHNHC_6H_5$	196.25	12, 236			138–141			s eth; v s chl
d755	1,3-Diphenylguanidine	$C_6H_5NHC(=NH)NHC_6H_5$	211.27	12, 369	1.13		148–150	dec 170		s alc, hot bz, chl

1,3-Dioxacyclohexane, d732
1,4-Dioxacyclohexane, d733
1,3-Dioxacyclopentane, d734
3,6-Dioxa-1,11-undecanediol, t430
(2,5-Dioxo-4-imidazolidinyl)urea, a71
1,3-Dioxolane-2-one, e132
Dipentyl ketone, u11
Diphenic acid, b141
Diphenolic acid, b205
Diphenyl, b138
Diphenylacetone, d767
Diphenylbenzenes, t7 thru t9
sym-Diphenylcarbazide, d746
Diphenyldiazene, a312
Diphenylenemethane, f2
Diphenylethanedione, b35
Diphenylethanedione dioxime, b36
1,2-Diphenylethene, s9
Diphenylethyne, d742
Diphenylglycolic acid, b37
Diphenylglyoxime, b36


d732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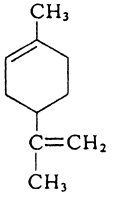
d734



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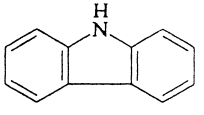


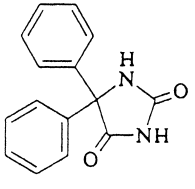
d751

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d756	5,5-Diphenylhydantoin		252.27	24, 410			294–297			i aq; 1.7 alc; 3.3 acet
d757	1,2-Diphenylhydrazine	$C_6H_5NHNHC_6H_5$	184.24	15, 123	1.158_4^{16}		123–126			v s alc; sl s bz
d758	Diphenylmercury	$(C_6H_5)_2Hg$	354.81	16, 946	2.318^4		128–129	dec >306		s chl; sl s hot alc
d759	Diphenylmethane	$C_6H_5CH_2C_6H_5$	168.24	5^2, 498	1.006	1.5768^{20}	25	265	>110	v s alc, bz, chl, eth
d760	Diphenylmethanol	$C_6H_5CH(OH)C_6H_5$	184.24	6, 678			66.7	298		0.05 aq; v s alc, chl, eth
d761	1,1-Diphenylmethylamine	$C_6H_5CH(NH_2)C_6H_5$	183.25	12, 1323	1.0635_4^{22}	1.5956^{99}	34	295	>112	sl s aq
d762	2,5-Diphenyloxazole		221.26	27, 78			72–74	360		
d763	Diphenyl phosphite	$(C_6H_5O)_2P(O)H$	234.19	6^1, 94	1.223	1.5575^{20}	12	219^{26mm}	176	
d764	Diphenylphosphoryl azide	$(C_6H_5O)_2P(O)N_3$	275.20		1.277	1.5518^{20}		$157^{0.17mm}$	>110	
d765	Diphenyl *o*-phthalate	$C_6H_4(CO_2C_6H_5)_2$	318.33	9, 801			74–76			
d766	2,2-Diphenyl-1-picrylhydrazyl		394.32	16^2, 363			127 dec			
d767	1,3-Diphenyl-2-propanone	$C_6H_5CH_2(C{=}O)CH_2C_6H_5$	210.28	7, 445	1.2		32–34	330		i aq; v s alc, eth
d768	2,2-Diphenylpropionic acid	$CH_3C(C_6H_5)_2CO_2H$	226.28	9^2, 474			175–177	300		s alc; v s bz, eth
d769	Diphenylsilanediol	$(C_6H_5)_2Si(OH)_2$	216.31	16, 909			140 dec		53	
d770	Diphenyl sulfide	$(C_6H_5)_2S$	186.28	6, 299	1.118_{15}^{15}	1.6327^{20}	−40	296	>110	misc bz, eth, CS_2
d771	Diphenyl sulfone	$(C_6H_5)_2SO_2$	218.27	6, 300			128–129	379		i aq; s hot alc, bz
d772	Diphenyl sulfoxide	$(C_6H_5)_2SO$	202.28	6, 300			69–71	207^{13mm}		
d773	Diphenylthiocarbazone	$C_6H_5N{=}NC(S)NHNHC_6H_5$	256.33	16, 26			168 dec			i aq; v s chl, CCl_4
d774	1,3-Diphenyl-2-thiourea	$C_6H_5NHC(S)NHC_6H_5$	228.32	12, 394	1.32		154			i aq; v s alc, eth
d775	1,3-Diphenylurea	$C_6H_5NHC(O)NHC_6H_5$	212.35	12, 352	1.239		238	260 dec		0.015 aq; s eth, HOAc
d776	Dipiperidinomethane		182.31		0.915	1.4820^{20}		123^{15mm}	91	
d777	Dipropylamine	$(C_3H_7)_2NH$	101.19	4, 138	0.7375_4^{20}	1.4043^{20}	−63	109.2	17	4 aq; v s alc, eth, PE
d778	3-Dipropylamino-1,2-propanediol	$(C_3H_7)_2NCH_2CH(OH)CH_2OH$	175.27	4^3, 841	0.949	1.4554^{20}		143^{9mm}	>110	
d779	Dipropylene glycol	$HO(CH_2)_3O(CH_2)_3OH$	134.18	1^2, 537	1.023	1.4410^{20}			137	
d780	Dipropylene glycol butyl ether	$CH_3CH(OH)CH_2OCH_2CH(OC_4H_9)CH_3$	190.29	1, *4*, 2474	0.917_{25}^{25}	1.425^{25}		229	96	

d781	Dipropylene glycol *tert*-butyl ether	$(CH_3)_3CO(CH_2)_3O(CH_2)_3OH$	190.29		0.900	1.4240^{20}		220–222	87	
d782	Dipropylene glycol dibenzoate	$[C_6H_5CO_2(CH_2)_3]_2O$	342.40	9^2, 108	1.120	1.5280^{20}		232^{5mm}	>110	
d783	Dipropylene glycol isopropyl ether	$CH_3CH(OH)CH_2OCH_2$-$CH[OCH(CH_3)_2]CH_3$	176.2		0.878^{25}_{25}	1.421^{25}		80.1	90	
d784	Dipropylene glycol methyl ether	$CH_3CH(OH)CH_2OCH_2$-$CH(OCH_3)CH_3$	148.2		0.951^{20}_{20}	1.419^{20}	−117	188.3	74	
d785	Dipropylene glycol acetate	$CH_3CO_2(CH_2)_3O(CH_2)_3$-$OCH_3$	190.24		0.970	1.4180^{20}		200	85	
d786	Dipropyl ether	$(C_3H_7)_2O$	102.18	1, 354	0.7466^{20}	1.3803^{20}	−126.2	89.6	21	0.4 aq
d787	Dipropyl hexanedioate	$C_3H_7O_2C(CH_2)_4CO_2C_3H_7$	230.30	2^2, 574	0.9790^{20}_4	1.4314^{20}	−20	144^{10mm}		i aq; s alc, eth
d788	Dipropyl sulfate	$(C_3H_7O)_2SO_2$	182.24	1, 354	1.106^{20}_4		dec 140	120^{20mm}		v s PE
d789	Dipropyl sulfone	$(C_3H_7)_2SO_2$	150.24	1, 359	1.028^{50}_4		28–30	270	126	
d790	2,2′-Dipyridyl		156.19	23, 199			70–73	273		0.5 aq; v s alc, bz, chl, eth, PE
d791	Disilane	H_3SiSiH_3	62.22	Merck: 12, 3419	0.686^{-25}_4		−132	−14.3	ignites in air	s alc, bz, CS_2

5,5-Diphenyl-2,4-imidazolidinedione, d756
Diphenyl ketone, b53
Diphenylmethanone, b53
1,1-Diphenylmethylamine, a159
Diphenyl oxide, d753
Diphenylphosphorochloridate, d748
1,3-Diphenyl-1,3-propanedione, d68
sym-Diphenylthiourea, t141
Dipicolinic acid, p270
Di-2-propenylamine, d30
Dipropyl adipate, d787
Dipropylene glycol, b204
Dipropyl ketone, h16
Distearylpentaerythritol diphosphite, b217
Disulfram, t62



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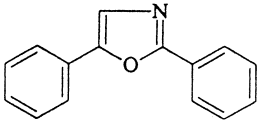

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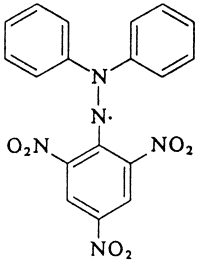
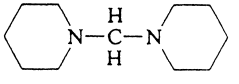


d766



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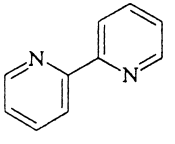


d790

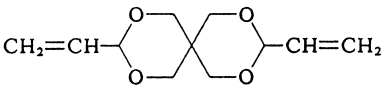
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
d792	1,3-Dithiane		120.24				53–55		90	
d793	4,4′-Dithiobutyric acid	$HO_2C(CH_2)_3SS(CH_2)_3CO_2H$	238.32	3, 312			110			
d794	3,3′-Dithiodipropionic acid	$HO_2C(CH_2)_2SS(CH_2)_2CO_2H$	210.27				157–159			
d795	Dithiooxamide	$H_2NC(S)C(S)NH_2$	120.20	2, 565			245			sl s aq; s alc; i eth
d796	2,2′-Dithiosalicylic acid	$S_2(C_6H_4CO_2H)_2$	306.36	10, 129			287–290			
d797	1,3-Di-*o*-tolylguanidine	$(CH_3C_6H_4NH)_2C{=}NH$	239.32	12, 803	1.10_4^{20}		176–178			s hot alc, eth
d798	Divinyl ether	$H_2C{=}CHOCH{=}CH_2$	70.09	Merck: 12, 10133	0.773_4^{20}	1.3989^{20}	−101	28.3	< −30	0.53 aq; misc alc, eth
d799	1,3-Divinyltetra-methyldisiloxane	$[CH_2{=}CHSi(CH_3)_2]_2O$	186.39	4,4,4080	0.811_4^{20}	1.4110^{20}	−99	139	24	
d800	3,9-Divinyl-2,4,8,10-tetraoxaspiro[5.5]-undecane		212.25	19^3, 5679	1.251		43–46	110^{2mm}	110	
d801	Docasane	$CH_3(CH_2)_{20}CH_3$	310.61	1, 174	0.7782^{45}	1.4358^{45}	43–45	369	>110	i aq; sl s alc; v s eth
d802	1-Docosanol	$CH_3(CH_2)_{21}OH$	326.61	1, 431			65–72	180^{22mm}		sl s eth; s alc, chl
d803	Dodecane	$CH_3(CH_2)_{10}CH_3$	170.34	1, 171	0.7490_4^{20}	1.4216^{20}	−10	216.2	74	
d804	1,12-Dodecanediamine	$H_2N(CH_2)_{12}NH_2$	200.37	4, 273			71		155	
d805	Dodecanedioic acid	$HO_2C(CH_2)_{10}CO_2H$	230.30	2, 729			128–130	245^{10mm}		
d806	1,2-Dodecanediol	$CH_3(CH_2)_9CH(OH)CH_2OH$	202.34	1^3, 2237			58–60			
d807	1,12-Dodecanediol	$HOCH_2(CH_2)_{10}CH_2OH$	202.34	1^2, 562			81–84	189^{12mm}		
d808	1-Dodecanethiol	$CH_3(CH_2)_{11}SH$	202.40		0.845_{20}^{20}	1.4587^{20}		266–283	87	i aq; s alc, eth
d809	Dodecanoic acid	$CH_3(CH_2)_{10}CO_2H$	200.32	2, 359	0.869^{14}	1.4183^{82}	43	225^{100mm}	>110	i aq; 100 alc; v s bz, eth; 40 PrOH
d810	1-Dodecanol	$CH_3(CH_2)_{11}OH$	186.34	1, 428	0.8308_4^{25}	1.4413^{25}	24	259	>110	i aq; s alc, eth
d811	δ-Dodecanolactone		198.31	17^5,9,100	0.942	1.4602^{20}	−12	126^{1mm}	>110	
d812	Dodecanoyl peroxide	$[CH_3(CH_2)_{10}CO]_2O_2$	398.63	2^3, 893			55–57			
d813	1-Dodecene	$CH_3(CH_2)_9CH{=}CH_2$	168.32	1, 225	0.7584_4^{20}	1.4294^{20}	−35.2	213.4	79	s alc, eth, PE
d814	2-Dodecen-1-ylsuccinic anhydride		266.38				41–43	180^{5mm}	177	
d815	Dodecyl acetate	$CH_3CO_2(CH_2)_{11}CH_3$	228.38	2, 136	0.865	1.4318^{20}		150^{15mm}	>110	
d816	Dodecyl acrylate	$H_2C{=}CHCO_2(CH_2)_{11}CH_3$	240.39	2^3, 1230	0.884	1.4450^{20}			>110	

d817	Dodecyl aldehyde	$CH_3(CH_2)_{10}CHO$	184.32	1, 714	0.835	1.4344^{20}		185^{100mm}	101	
d818	Dodecylamine	$CH_3(CH_2)_{11}NH_2$	185.36	4, 200	0.808		30–32	247–249	>110	misc alc, bz, chl, eth
d819	Dodecyl methacrylate	$H_2C{=}C(CH_3)CO_2(CH_2)_{11}CH_3$	254.42	2^3, 1290	0.868	1.4460^{20}	−7	142^{4mm}	>110	
d820	Dodecyl sulfate, sodium salt	$CH_3(CH_2)_{11}SO_3^-\ Na^+$	288.38	1^3, 1786			204–207			10 aq
d821	Dodecyltrichlorosilane	$CH_3(CH_2)_{11}SiCl_3$	303.8	4^3, 1907	1.020	1.458^{20}		294	>110	
d822	Dodecyl vinyl ether	$CH_3(CH_2)_{11}OCH{=}CH_2$	212.38		0.817	1.4382^{20}		117–120	>110	
d823	Dotriacontane	$CH_3(CH_2)_{30}CH_3$	450.88	1,177	0.8124_4^{20}	1.4364^{70}	68–70	467		sl s alc, bz, eth
d824	Dulcitol		182.17	1, 544	1.47^{20}		188–191	280^{1mm}		3.3 aq; sl s alc
e1	Eicosane	$CH_3(CH_2)_{18}CH_3$	282.56	1, 174	0.7823 (s)		37	343	>110	
e2	1*R*,2*S*-(−)-Ephedrine	$CH_3NHCH(CH_3)CH(OH)C_6H_5$	165.24	13, 636	1.124		39	255	85	s aq, alc, chl, eth
e3	1,2-Epoxybutane		72.11	17^2, 17	0.8297^{20}	1.3850^{20}	−150	63	−22	6 aq; misc alc, bz, chl, eth

2,3-Dithiabutane, d607
5,6-Dithiadecane, d146
3,4-Dithiahexane, d356
2,2′-Dithiodibenzoic acid, d796
2,2′-Dithiodiethanol, h123
Dithizone, d773
Divinylene oxide, f45
DMSO, d697
Dodecyl alcohol, d810
Dodecyl iodide, i30
DPPH, d766
Durene, t99
EDTA, e134
Eicosane, i1
1-Eicosene, i2
Elaidic acid, o11
Enanthic alcohol, h11
Enanthylic acid, h9
Epibromohydrin, b328
Epichlorohydrine, c120
1,4-Epoxybutane, t69


d792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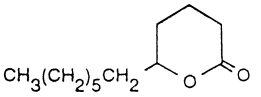
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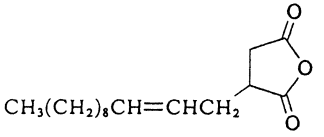
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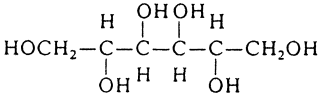
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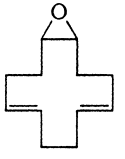
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
e4	1,2-Epoxy-5,9-cyclo-dodecadiene		178.28		0.980	1.5045^{20}		83^{1mm}	>110	
e5	1,2-Epoxycyclo-dodecane		182.31		0.939	1.4773^{20}			>110	
e6	1,2-Epoxycyclopentane		84.12	17, 21	0.964	1.4336^{20}		102	10	
e7	1,2-Epoxydecane	$H_2C(O)CHCH_2(CH_2)_6CH_3$	156.27	17, 18	0.840	1.4290^{20}		94^{15mm}	78	
e8	1,2-Epoxydodecane	$H_2C(O)CHCH_2(CH_2)_8CH_3$	184.32	17[3], 136	0.844	1.4355^{20}		125^{15mm}	105	
e9	1,2-Epoxyethylbenzene	$H_2C(O)CHC_6H_5$	120.15	17, 49	1.0523_4^{16}	1.5338^{20}	−37	194	79	i aq; s alc, eth
e10	1,2-Epoxyhexadecane	$H_2C(O)CHCH_2(CH_2)_{12}CH_3$	240.43	17, 20	0.846	1.4452^{20}	21–22	180^{12mm}	93	
e11	1,2-Epoxyhexane	$H_2C(O)CHCH_2CH_2CH_2CH_3$	100.16	17[4], 86	0.831	1.4056^{20}		118–120	15	
e12	1,2-Epoxy-5-hexene	$H_2C(O)CHCH_2CH_2CH{=}CH_2$	98.15	17[3], 163	0.870	1.4252^{20}		121	15	
e13	1,2-Epoxyoctadecane	$H_2C(O)CHCH_2(CH_2)_{14}CH_3$	268.49	17[3], 140			33–35	$137^{0.5mm}$	>110	
e14	1,2-Epoxy-3-phenoxy-propane	$H_2C(O)CHCH_2OC_6H_5$	150.18	17, 105	1.109	1.530^{20}	3.5	245	>110	
e15	1,2-Epoxypropane	$H_2C(O)CHCH_3$	58.08	17, 6	0.859_4^0	1.3660^{20}	−112	35	−37	41 aq; misc alc, eth
e16	2,3-Epoxy-1-propanol	$H_2C(O)CHCH_2OH$	74.08	17, 104	1.1143_4^{25}	1.4315^{20}		$66^{2.5mm}$	81	misc aq
e17	2,3-Epoxypropyl-methacrylate	$H_2C(O)CHCH_2O_2C(CH_3)$-$CH{=}CH_2$	142.16		1.042	1.4494^{20}		189	76	

e18	1,2-Epoxy-3,3,3-trichloropropane	$H_2C(O)CHCCl_3$	161.42	17^{2}, 14	1.495	1.4778^{20}		151^{745mm}	66	
e19	*meso*-Erythritol	$HOCH_2[CH(OH)]_2CH_2OH$	122.12	1, 525			120–123	329–331		
e20	Ethane	CH_3CH_3	30.07	1, 80	1.356^{0} g/L		−182.8	−88	−135	4.7 mL aq; 46 mL alc[4]
e21	1,2-Ethanediamine	$H_2NCH_2CH_2NH_2$	60.10	4, 230	0.8977_4^{20}	1.4568^{20}	11	117.3	33	misc aq, alc; i bz
e21a	1,2-Ethanediol	$HOCH_2CH_2OH$	62.07	1, 465	1.1135_4^{20}	1.4318^{20}	−12.6	197.3	110	misc aq, alc, glyc, pyr
e22	1,2-Ethanediol diacetate	$CH_3CO_2CH_2CH_2O_2CCH_3$	146.14	2, 142	1.1043^{20}	1.4150^{20}	−31	190.2	82	misc alc, eth
e23	1,2-Ethanediol dimethacrylate	$[H_2C{=}C(CH_3)CO_2CH_2^-]_2$	198.22	2^{3}, 1292	1.051	1.4549^{20}		100^{5mm}	>110	
e24	1,2-Ethanedithiol	$HSCH_2CH_2SH$	94.20	1, 471	1.123^{24}	1.5580^{20}		146	50	v s alc, alk
e25	Ethanesulfonic acid	$C_2H_5SO_3H$	110.13	4, 5	1.350	1.4340^{20}	−17	$123^{0.01mm}$	>110	
e26	Ethanesulfonyl chloride	$CH_3CH_2SO_2Cl$	128.57	4, 6	1.357^{22}	1.4330^{20}		177	83	dec aq, alc; v s eth
e26a	Ethanethiol	CH_3CH_2SH	62.13	1, 340	0.8315^{25}	1.420^{25}	−147.9	35.0	−17	0.7 aq; s alc, eth
e27	Ethanol	CH_3CH_2OH	46.07	1, 292	0.7894_4^{20}	1.3611^{20}	−114	78.3	13	misc aq, alc, chl, eth
e28	Ethanol-*d*	CH_3CH_2OD	47.08	1^{3}, 1287	0.801	1.3595^{20}		78.8	12	misc aq, alc, eth
e29	Ethanolamine	$H_2NCH_2CH_2OH$	61.08	Merck: 12, 3712	1.0180^{20}	1.4539^{20}	10.5	170.8	86	misc aq, alc, acet
e30	Ethoxyacetic acid	$CH_3CH_2OCH_2CO_2H$	104.11	3, 233	1.1021_4^{20}	1.4190^{20}		97^{11mm}	97	s aq, alc, eth

Epoxyethane, e147
1,2-Epoxy-1-methoxy-2-methylpropane, m86
1,2-Epoxypropane, p232
Estragole, a89
Ethanal, a4
Ethanamide, a6
Ethanamidine HCl, a7
Ethanedial, g28
1,2-Ethanediol, e135
Ethanediamide, o58
Ethanenitrile, a29
Ethanoic acid, a19
Ethanoic anhydride, a22
Ethanolamine, a164
Ethanoyl bromide, a35
Ethanoyl chloride, a37
Ethene, e131
Ethenone, k1
Ethenyl acetate, v2
Ethenylbenzene, s11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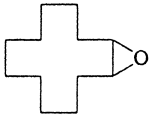
e5

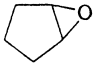
e6

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
e31	3-Ethoxyacrylonitrile	$C_2H_5OCH{=}CHCN$	97.12	3^3, 681	0.944	1.4545^{20}		91^{19mm}	81	
e32	4-Ethoxyaniline	$CH_3CH_2OC_6H_5NH_2$	137.18	13, 436	1.0652^{16}_4	1.5609^{20}	4	250	115	i aq; s alc
e33	2-Ethoxybenzaldehyde	$CH_3CH_2OC_6H_4CHO$	150.18	8, 43	1.074	1.5422	20	136^{24mm}	107	misc alc, eth
e34	4-Ethoxybenzaldehyde	$CH_3CH_2OC_6H_4CHO$	150.18	8, 73	1.080^{25}_{25}	1.5584^{20}	13–14	255	>110	v s alc, bz, eth
e35	2-Ethoxybenzamide	$CH_3CH_2OC_6H_4CONH_2$	165.19	10, 93			132–134			sl s aq; s alc, eth
e36	Ethoxybenzene	$CH_3CH_2OC_6H_5$	122.17	6, 140	0.967^{20}_4	1.5074^{20}	−29.5	169.8	63	v s alc, eth
e37	2-Ethoxybenzoic acid	$CH_3CH_2OC_6H_4CO_2H$	166.18	10, 64	1.105	1.5400^{20}	19.4	174^{15mm}	>110	sl s aq
e38	4-Ethoxybenzoic acid	$CH_3CH_2OC_6H_4CO_2H$	166.18	10, 156			197–199			sl s hot aq
e39	Ethoxycarbonyl isothiocyanate	$CH_3CH_2OC(=O)NCS$	131.15	3^3, 279	1.112	1.5000^{20}		56^{18mm}	50	
e40	2-Ethoxyethanol	$CH_3CH_2OCH_2CH_2OH$	90.12	1, 467	0.9295^{20}	1.4075^{20}	−70	134.8	43	misc aq, alc, acet, eth
e41	2-(2-Ethoxyethoxy)-ethanol	$C_2H_5OCH_2CH_2OCH_2CH_2OH$	134.18	1^2, 520	0.9841^{25}_4	1.4254^{25}	−76	196	96	misc aq, alc, bz, chl, acet, pyr
e41a	2-(2-Ethoxyethoxy)-ethanol acetate	$CH_3CO_2CH_2CH_2OCH_2CH_2$-$OCH_2CH_3$	176.21		1.0096^{20}	1.4213^{20}	−25	218.5	110	
e42	2-Ethoxyethyl acetate	$CH_3CO_2CH_2CH_2OCH_2CH_3$	132.16	2^2, 155	0.9749^{20}_4	1.4023^{20}	−61.7	156.3	57	29 aq; misc alc, eth
e43	2-Ethoxyethyl acrylate	$H_2C{=}CHCO_2CH_2CH_2OC_2H_5$	144.17	2^3, 1232	0.982	1.4270^{20}		78^{23mm}	65	
e44	2-Ethoxyethylamine	$CH_3CH_2OCH_2CH_2NH_2$	89.14	4^2, 718	0.8512^{20}_4	1.4101^{20}		107	21	misc aq, alc, eth
e45	2-Ethoxyethyl methacrylate	$H_2C{=}C(CH_3)CO_2CH_2CH_2OC_2H_5$	158.20	2^3, 1291	0.964	1.4285^{20}		93^{35mm}	71	
e46	3-Ethoxy-4-hydroxy-benzaldehyde	$C_2H_5OC_6H_3(OH)CHO$	166.18	8, 256			76–78			s eth, glycols; 50 alc
e47	3-Ethoxy-4-methoxy-benzaldehyde	$C_2H_5OC_6H_3(OCH_3)CHO$	180.2	8, 256			51–53		>110	s alc, bz, chl, eth
e48	1-Ethoxy-2-methoxy-benzene	$C_2H_5OC_6H_4OCH_3$	152.19	6, 771	1.044	1.5240^{20}		217–218	90	
e49	Ethoxymethylene-malononitrile	$CH_3CH_2OCH{=}C(CN)_2$	122.13	3^1, 162			64–66	160^{12mm}		
e50	1-Ethoxynaphthalene	$C_{10}H_7OCH_2CH_3$	172.23	6, 606	1.060^{20}_4	1.6040^{20}	5.5	280	>110	i aq; v s alc, eth
e51	2-Ethoxyphenol	$C_2H_5OC_6H_4OH$	138.17	6, 771	1.090	1.5288^{20}	29	217	91	
e52	*trans*-2-Ethoxy-5-(1-propenyl)phenyl	$C_2H_5OC_6H_3(CH{=}CHCH_3)OH$	178.23	6^2, 918			86–88			
e53	3-Ethoxypropionitrile	$C_2H_5OCH_2CH_2CN$	99.14	3, 298	0.911	1.4065^{20}		171–172	63	

e54	3-Ethoxypropylamine	$C_2H_5OCH_2CH_2CH_2NH_2$	103.17	4^3, 739	0.861	1.4178^{20}		136–138	32	
e55	3-Ethoxysalicyl-aldehyde	$C_2H_5OC_6H_3(OH)CHO$	166.18	8^2, 267			66–68	264		
e56	Ethoxytrimethylsilane	$(CH_3)_3SiOC_2H_5$	118.3	4^3, 1856	0.7573_4^{20}	1.3742^{20}		75–76	−18	
e57	Ethyl acetate	$CH_3CO_2C_2H_5$	88.11	2, 125	0.9006_4^{20}	1.3724^{20}	−84	77	−4	9.7 aq; misc alc, acet, chl, eth
e58	Ethyl acetoacetate	$CH_3COCH_2CO_2C_2H_5$	130.15	3, 632	1.0213_4^{25}	1.4174^{20}	−45	180.8	57	2.9 aq; misc alc, chl
e59	*p*-Ethylacetophenone	$C_2H_5C_6H_4COCH_3$	148.21	7^4, 1101	0.993	1.5293^{20}	−20.6	114^{11mm}	90	
e60	Ethyl acrylate	$H_2C{=}CHCO_2C_2H_5$	100.12	2, 399	0.9234^{20}	1.4060^{20}	−71	99	10	1.5 aq; s alc, eth
e61	Ethylaluminum dichloride	$C_2H_5AlCl_2$	126.95	4^3, 1973	1.207^{50}		32	113^{50mm}	−18	
e62	Ethylaluminum sesquichloride	$C_2H_5AlCl_2 \cdot ClAl(C_2H_5)_2$	247.51		1.092		−50	204	−18	
e63	Ethylamine	$C_2H_5NH_2$	45.09	4, 87	0.689_{15}^{15}	1.3663^{20}	−81	16.6	< −18	misc aq, alc, eth
e64	Ethyl 2-aminobenzoate	$H_2NC_6H_4CO_2C_2H_5$	165.19	14, 319	1.088^{15}	1.5640^{20}	13–15	266–268	>110	i aq; s alc, eth
e65	Ethyl 4-aminobenzoate	$H_2NC_6H_4CO_2C_2H_5$	165.19	14, 422			88–90	310		0.04 aq; 20 alc; 50 chl, 25 eth; s dil acid
e66	Ethyl 3-amino-crotonate	$CH_3C(NH_2){=}CHCO_2C_2H_5$	129.16	3, 654	1.021_4^{20}		33–35	210–215	97	i aq; s alc, bz, eth
e67	2-(Ethylamino)ethanol	$CH_3CH_2NHCH_2CH_2OH$	89.14	4, 282	0.914_4^{20}	1.4402^{20}	−90	170	71	v s aq, alc, eth
e68	*N*-Ethylaniline	$C_6H_5NHC_2H_5$	121.18	12, 159	0.958_{25}^{25}	1.5559^{20}	−63.5	203	85	i aq; misc alc, eth
e69	2-Ethylaniline	$CH_3CH_2C_6H_4NH_2$	121.18	12^2, 584	0.983	1.5590^{20}	−44	210	91	sl s aq; v s alc, eth
e70	4-Ethylaniline	$CH_3CH_2C_6H_4NH_2$	121.18	12, 1090	0.975	1.5542^{20}	−5	216	85	sl s aq; v s alc, eth
e71	2-Ethylanthraquinone		236.27	7^1, 425			108–111			
e72	4-Ethylbenzaldehyde	$C_2H_5C_6H_4CHO$	134.18	7, 307	0.979	1.5390^{20}		221	92	
e73	Ethylbenzene-d_{10}	$C_6D_5CD_2CD_3$	116.25		0.949	1.4920^{20}		134.6	31	

4-Ethoxy-*m*-anisaldehyde, e48
1-Ethoxybutane, b554
Ethoxyethane, d365
2-Ethoxyethyl ether, b186
Ethoxyformic anhydride, d386
(Ethoxymethyl)benzene, b97
α-Ethoxy-*α*-phenylacetophenone, b47
3-Ethoxy-1-propene, a86
Ethylacetylene, b160a
Ethyl alcohol, e27, e28
Ethylaldehyde, a4
Ethyl anthranilate, e64
Ethyl benzencarboxylate, e76

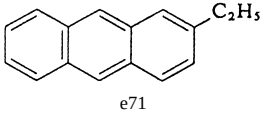

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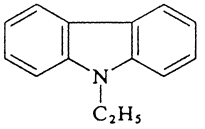
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
e74	Ethylbenzene	$C_6H_5CH_2CH_3$	106.17	5^2, 274	0.8670_4^{20}	1.4959^{20}	−95.0	136.2	22	0.01 aq; misc alc, bz, chl, eth
e75	4-Ethylbenzene-sulfonic acid	$C_2H_5C_6H_4SO_3H$	186.23	11, 120	1.229	1.5331			>110	
e76	Ethyl benzoate	$C_6H_5CO_2C_2H_5$	150.18	9, 110	1.051^{15}	1.5000^{20}	−34.7	212.4	84	0.05 aq; misc alc, chl, bz, eth, PE
e77	Ethyl benzoylacetate	$C_6H_5(C{=}O)CH_2CO_2C_2H_5$	192.21	10, 674	1.110	1.5338^{20}		265–270	63	i aq; misc alc, eth
e78	Ethyl 3-benzoyl-acrylate	$C_6H_5(C{=}O)CH{=}CHCO_2C_2H_5$	204.23	10^2, 501	1.112	1.5435^{20}		185^{25mm}	>110	
e79	Ethyl 2-benzylaceto-acetate	$CH_3C(=O)CH(CH_2C_6H_5)CO_2C_2H_5$	220.27	10, 710	1.036	1.4996^{20}		276	>110	
e80	*N*-Ethylbenzylamine	$C_6H_5CH_2NHC_2H_5$	135.21	12, 1020	0.909	1.5117^{20}		194	66	
e81	Ethyl (2-benzyl)-benzoylacetate	$C_6H_5C(=O)CH(CH_2C_6H_5)$-$CO_2C_2H_5$	282.34	10, 764	1.110	1.5567^{20}		270^{80mm}	>110	
e82	Ethyl *N*-benzyl-*N*-cyclopropylcarba-mate	$C_6H_5CH_2N(C_3H_5)CO_2C_2H_5$	219.28		0.997	1.5104^{20}			>110	
e83	Ethyl bromoacetate	$BrCH_2CO_2CH_2CH_3$	167.01	2, 214	1.506_{20}^{20}	1.4510^{20}	< −20	159	47	i aq; misc alc, eth
e84	Ethyl 4-bromo-benzoate	$BrC_6H_4CO_2C_2H_5$	229.08	9, 352	1.403	1.5440^{20}		131^{14mm}	>110	
e85	Ethyl 2-bromobutyrate	$CH_3CH_2CH(Br)CO_2C_2H_5$	195.06	2^2, 255	1.329_{20}^{20}	1.4470^{20}		177 dec	58	i aq; misc alc, eth
e86	Ethyl 4-bromobutyrate	$BrCH_2CH_2CH_2CO_2C_2H_5$	195.06	2, 283	1.363	1.4559^{20}		82^{10mm}	90	
e87	Ethyl 2-bromo-heptanoate	$CH_3(CH_2)_3CH(Br)CO_2C_2H_5$	237.14	2, 341	1.211	1.4524^{20}		109^{10mm}	104	
e88	Ethyl 6-bromo-hexanoate	$Br(CH_2)_5CO_2C_2H_5$	223.12	2^3, 737	1.254	1.4590^{20}		130^{16mm}	>110	
e89	Ethyl 2-bromoiso-butyrate	$(CH_3)_2C(Br)CO_2C_2H_5$	195.06	2, 296	1.329_4^{20}	1.4446^{20}		67^{11mm}	60	i aq; misc alc, eth
e90	Ethyl 2-bromo-octanoate	$CH_3(CH_2)_5CH(Br)CO_2C_2H_5$	251.17	2, 349	1.167	1.4520^{20}			106	
e91	Ethyl 3-bromo-2-oxo-propionate	$BrCH_2C(=O)CO_2C_2H_5$	195.02	3^2, 409	1.554	1.4695^{20}		100^{10mm}	98	

e92	Ethyl 2-bromo-pentanoate	$CH_3(CH_2)_2CH(Br)CO_2C_2H_5$	209.09	2, 302	1.116	1.4486^{20}		190–192	77	i aq; misc alc, eth
e93	Ethyl 2-bromo-propionate	$CH_3CH(Br)CO_2C_2H_5$	181.03	2, 255	1.394	1.4460^{20}		156–160	51	i aq; misc alc, eth
e94	Ethyl 3-bromo-propionate	$BrCH_2CH_2CO_2C_2H_5$	181.03	2, 256	1.4123_4^{18}	1.4569^{18}		136^{50mm}	79	i aq; misc alc, eth
e95	2-Ethyl-1-butanol	$(C_2H_5)_2CHCH_2OH$	102.18	1, 412	0.8330^{20}	1.4224^{20}	< -15	146	58	0.63 aq
e95a	2-Ethyl-1-butene	$(C_2H_5)_2C{=}CH_2$	84.16	1[2], 95	0.689	1.3960^{20}	−131	65	−26	
e96	2-Ethylbutyl acetate	$CH_3CO_2CH_2CH(C_2H_5)_2$	144.21	2[3], 257	0.876	1.4100^{20}		160^{740mm}	52	
e97	*N*-Ethylbutylamine	$CH_3(CH_2)_3NHC_2H_5$	101.19	4, 157	0.740_4^{20}	1.4050^{20}		108	18	
e98	2-Ethylbutyraldehyde	$(C_2H_5)_2CHCHO$	100.16	1, 693	0.8162_{20}^{20}	1.4018^{20}	−89	116.7	21	0.31 aq
e99	Ethyl butyrate	$CH_3CH_2CH_2CO_2C_2H_5$	116.16	2, 270	0.879_4^{20}	1.3998^{20}	−98	121	24	0.49 aq; misc alc, eth
e100	2-Ethylbutyric acid	$(C_2H_5)_2CHCO_2H$	116.16	2, 333	0.9225_{20}^{20}	1.4133^{20}	−14	194	87	
e101	Ethyl butyrylacetate	$CH_3(CH_2)_2C(=O)CH_2$-$CO_2C_2H_5$	158.20	3, 684	1.001	1.4270^{20}		104^{22mm}	78	
e102	Ethyl carbamate	$H_2NCO_2C_2H_5$	89.09	3, 22	1.056		49–50	182–184	92	200 aq; 125 alc; 111 chl; 67 eth
e103	Ethyl carbazate	$H_2NNHCO_2C_2H_5$	104.11	3, 98			44–47	110^{22mm}	86	
e104	*N*-Ethylcarbazole		195.27	20, 436			68–70			
e105	Ethyl chloroacetate	$ClCH_2CO_2C_2H_5$	122.55	2, 197	1.1498_4^{20}	1.4227^{20}	−21	144	65	i aq; misc alc, eth
e106	Ethyl 2-chloro-acetoacetate	$CH_3C(=O)CH(Cl)CO_2C_2H_5$	164.59	3, 662	1.190	1.4430^{20}		107^{14mm}	50	i aq; s alc, eth
e107	Ethyl 4-chloro-acetoacetate	$ClCH_2C(=O)CH_2CO_2C_2H_5$	164.59	3, 663	1.218_4^{17}	1.4520^{20}		115^{14mm}	96	i aq; misc alc, eth

Ethyl 3-benzenepropenoate, e113
α-Ethylbenzyl alcohol, p145
Ethyl benzyl ether, b97
Ethyl bromide, b329
Ethyl 2-bromo-2-methylpropanoate, e89
Ethyl bromopyruvate, e91
Ethyl bromovalerate, e92
Ethyl butanoate, e99
2-Ethylbutyl alcohol, e95
Ethyl butyl ether, b554
Ethyl butyl ketone, h15
Ethyl caprate, e120
Ethyl caproate, e160
Ethyl caprylate, e231
Ethyl chloride, c121



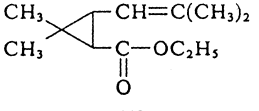
e104

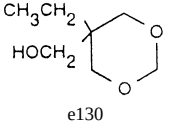
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
e108	Ethyl 4-chlorobutyrate	$ClCH_2CH_2CH_2CO_2C_2H_5$	150.61	2, 278	1.0754_4^{20}	1.4306^{20}		186	51	s alc, acet, eth
e109	Ethyl chloroformate	$ClCO_2C_2H_5$	108.52	3, 10	1.1403_4^{20}	1.3941^{20}	−81	93	13	misc alc, bz, chl, eth
e110	Ethyl 2-chloro-propionate	$CH_3CH(Cl)CO_2C_2H_5$	136.58	2, 248	1.087_4^{20}	1.4185^{20}	146–149	38		
e111	Ethyl 3-chloro-propionate	$ClCH_2CH_2CO_2C_2H_5$	136.58	2, 250	1.1086_4^{20}	1.4249^{20}		162–163	54	misc alc, eth
e112	Ethyl chrysanthemumate		196.29	9^2, 45	0.906	1.4600^{20}		112^{10mm}	84	
e113	Ethyl *trans*-cinnamate	$C_6H_5CH{=}CHCO_2C_2H_5$	176.22	9^2, 385	1.0495_4^{20}	1.5598^{20}	10	271	>110	misc alc, eth; i aq
e114	Ethyl crotonate	$CH_3CH{=}CHCO_2C_2H_5$	114.14	2, 411	0.9175_4^{20}	1.4240^{20}		138	28	i aq; s alc, eth
e115	Ethyl cyanoacetate	$NCCH_2CO_2C_2H_5$	113.12	2, 585	1.0564_4^{25}	1.4176^{20}	−22	206	110	i aq; misc alc, eth
e116	Ethyl 2-cyano-3,3-diphenylacrylate	$(C_6H_5)_2C{=}C(CN)CO_2C_2H_5$	277.33	9^3, 4601			97–99	$174^{0.2mm}$		
e117	Ethylcyclohexane	$C_6H_{11}CH_2CH_3$	112.22	5, 35	0.7879^{20}	1.4330^{20}	−111	131.8	35	
e118	4-Ethylcyclohexanol	$CH_3CH_2C_6H_{10}OH$	128.22	6^2, 26	0.889	1.4625^{20}		84^{10mm}	77	
e118a	Ethylcyclopentane	$C_2H_5(C_5H_9)$	98.19	5^2, 19	0.763	1.4190^{20}	−138	103	15	
e119	Ethyl cyclopropane-carboxylate	$C_3H_5CO_2CH_2CH_3$	114.14	9, 4	0.960	1.4197^{20}		129–133	18	
e120	Ethyl decanoate	$CH_3(CH_2)_8CO_2C_2H_5$	200.32	2, 356	0.862^{20}	1.4248^{20}		245	102	misc alc, chl, eth
e121	Ethyl diazoacetate	$N_2CH_2CO_2C_2H_5$	114.10	3^1, 211	1.0852_4^{18}	1.4588^{18}	−22	141^{710mm}	26	misc alc, bz, eth
e122	Ethyl 2,3-dibromo-propionate	$BrCH_2CH(Br)CO_2C_2H_5$	259.94	2, 259	1.788_4^{16}	1.4986^{20}		214	91	s alc, eth
e123	Ethyl dichloro-phosphate	$CH_3CH_2OP(O)Cl_2$	162.94	1, 332	1.373	1.4338^{20}		65^{10mm}	>110	
e124	Ethyl dichlorothio-phosphate	$CH_3CH_2OP(S)Cl_2$	179.01	1, 353	1.353	1.5040^{20}		68^{10mm}	>110	
e125	*N*-Ethyldiethanolamine	$CH_3CH_2N(CH_2CH_2OH)_2$	133.19	4, 284	1.014	1.4665^{20}	−50	246–252	123	
e126	Ethyl 3,3-dimethyl-acrylate	$(CH_3)_2C{=}CHCO_2C_2H_5$	128.17	2, 433	0.9247_4^{20}	1.4350^{20}		155	33	
e127	Ethyl 4-dimethyl-aminobenzoate	$(CH_3)_2NC_6H_4CO_2C_2H_5$	193.25	14^1, 571			64–66			
e128	Ethyl 2,2-dimethyl-propionate	$(CH_3)_3CCO_2C_2H_5$	130.19	2, 320	0.8584_4^{18}	1.3922^{18}		118.2	16	s alc, eth

e129	Ethyl 3,5-dinitrobenzoate	$(O_2N)_2C_6H_3CO_2C_2H_5$	240.17	9, 414			94–95			
e130	5-Ethyl-1,3-dioxane-5-methanol		146.19	19^{5},2,382	1.090	1.4630^{20}		105^{5mm}	>110	
e131	Ethylene	$H_2C{=}CH_2$	28.05	1, 180	1.147 g/L		−169.4	−104		11 mL aq[25]; 200 alc[25]; v s eth; s acet, bz
e132	Ethylene carbonate		88.06	19, 100	1.3214^{39}	1.4199^{40}	36.4	248	143	misc aq
e133	Ethylenediamine	$H_2NCH_2CH_2NH_2$	60.10	4, 230	0.879^{20}	1.4566^{20}	11	117	40	
e134	Ethylenediamine-*N*,*N*,*N*′,*N*′-tetraacetic acid	$(HO_2CCH_2)_2NCH_2CH_2N(CH_2CO_2H)_2$	292.24	4^{3}, 1187			250 dec			0.05 aq
e135	Ethylene glycol	$HOCH_2CH_2OH$	62.07	1, 465	1.113	1.4310^{20}		196–198	>110	
e136	Ethylene glycol bis(mercaptoacetate)	$(HSCH_2CO_2CH_2{-})_2$	210.27		1.313	1.5211^{20}		139^{2mm}	>110	
e137	Ethylene glycol diacetate	$CH_3CO_2CH_2CH_2O_2CCH_3$	146.14	2, 142	1.1043^{20}	1.4159^{20}	−31	190	88	
e138	Ethylene glycol diethyl ether	$C_2H_5OCH_2CH_2OC_2H_5$	118.18	1, 468	0.8484^{20}	1.3860^{20}	−74	119	35	
e139	Ethylene glycol diglycidyl ether	$(H_2C(O)CHCH_2OCH_2{-})_2$	174.20	1, 468	0.842	1.3923^{20}	−74	121	20	
e140	Ethylene glycol dimethacrylate	$[H_2C{=}C(CH_3)CO_2CH_2{-}]_2$	198.22	2^{3}, 1292	1.051	1.4549^{20}		100^{5mm}	>110	

Ethyl chloroglyoxylate, e232
Ethyl citrate, t278
Ethyl cyanide, p215
Ethyl 2-cyano-3-ethoxyacrylate, e150
N-Ethyldiisopropylamine, d477
Ethylene bromohydrin, b331
Ethylene chlorobromide, b303
Ethylene chlorohydrin, c122
Ethylene cyanohydrin, h173
Ethylene diacetate, e22
Ethylenediamine, e21
Ethylene dibromide, d97
Ethylene dichloride, d226
Ethylene diglyme, b186
(Ethylenedinitril)tetraacetic acid, e134
2,2′-Ethylenedioxybis(ethanol), t280
Ethylene glycol, e21a
Ethylene glycol bis(thioglycolate), e136
Ethylene glycol *tert*-butyl ether, b494
Ethylene glycol *tert*-butyl methyl ether, b498
Ethylene glycol *p*-butylphenyl ether, b590
Ethylene glycol diacetate, e22
Ethylene glycol diethyl ether, d304
Ethylene glycol dimethacrylate, e23


e112


e130

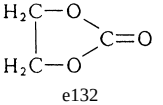
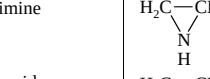
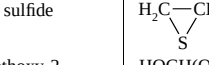
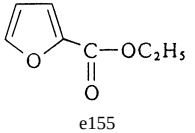

e132

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
e141	Ethylene glycol dimethyl ether	$CH_3OCH_2CH_2OCH_3$	90.12	1, 467	0.8691^{20}	1.3796^{20}	−58	85	−2	
e142	Ethylene glycol divinyl ether	$H_2C{=}CHOCH_2CH_2OCH{=}CH_2$	114.14	1^3, 2807	0.914	1.4350^{20}		125–127	27	
e143	Ethylene glycol methyl ether acrylate	$H_2C{=}CHCO_2CH_2CH_2OCH_3$	130.14	2^3, 1232	1.012	1.4270^{20}		56^{12mm}	60	
e144	Ethylene glycol methyl ether methacrylate	$H_2C{=}C(CH_3)CO_2CH_2CH_2OCH_3$	144.17	2^3, 1291	0.993	1.4310^{20}		65^{12mm}	60	
e145	Ethylene glycol phenyl ether acrylate	$H_2C{=}CHCO_2CH_2CH_2OC_6H_5$	192.21	6^3, 572	1.104	1.5180^{20}		$84^{0.2mm}$	>110	
e146	Ethyleneimine		43.07		0.8321_4^{25}	1.4123^{25}	−78	56	−11	misc aq; s alc
e147	Ethylene oxide		44.05	17, 4	0.891_4^0	1.3597^7	−111	10.6	−18	misc aq; s alc, eth
e148	Ethylene sulfide		60.12	17^2, 12	1.010	1.4935^{20}		55–56	10	sl s alc, eth
e149	Ethyl 2-ethoxy-2-hydroxyacetate	$HOCH(OC_2H_5)CO_2C_2H_5$	148.16	3, 601	1.079	1.4200^{20}		137	49	
e150	Ethyl (ethoxy-methylene)cyano-acetate	$C_2H_5OCH{=}C(CN)CO_2C_2H_5$	169.18	3, 470			51–53	190^{30mm}	>110	
e151	Ethyl 3-ethoxy-propionate	$C_2H_5OCH_2CH_2CO_2C_2H_5$	146.19	3, 298	0.949	1.4050^{20}		166	52	
e152	Ethyl 4-{[(ethyl-phenylamino)-methylene]amino}-benzoate	$C_6H_5N(C_2H_5)CH{=}N{-}C_6H_4$-$CO_2C_2H_5$	296.37				62–65	215^{2mm}		
e153	Ethyl fluoroacetate	$FCH_2CO_2C_2H_5$	106.10	2, 193	1.0926^{21}	1.3755^{20}		119	30	s aq
e154	Ethyl formate	$HCO_2C_2H_5$	74.08	2, 19	0.917_4^{20}	1.3590^{20}	−80	54	−20	10 aq; misc alc, eth
e155	Ethyl 2-furoate		140.14	18, 275	1.117_4^{20}		35–37	196	70	i aq; s alc, eth
e156	Ethyl heptanoate	$CH_3(CH_2)_5CO_2C_2H_5$	158.24	2^2, 295	0.8685_4^{20}	1.4144^{15}	−66	189	66	s alc, eth

e157	Ethyl hexadecanoate	$CH_3(CH_2)_{14}CO_2C_2H_5$	284.48	2^2, 336	0.8577^{25}_4	1.4347^{34}	22	191^{10mm}		s alc, eth
e158	2-Ethylhexanaldehyde	$CH_3(CH_2)_3CH(C_2H_5)CHO$	128.22	1, 707	0.822	1.4155		$55^{13.5mm}$	42	
e158a	3-Ethylhexane	$(C_2H_5)CHCH_2CH_2CH_3$	114.23	1^4, 431	0.7136^{20}	1.4018^{20}		118.6		s alc, eth
e159	2-Ethyl-1,3-hexanediol	$CH_3(CH_2)_2CH(OH)$-$CH(C_2H_5)CH_2OH$	146.23	Merck: 12, 3790	0.9325^{22}_4	1.4530^{22}	−40	244	127	0.6% (w/w) aq; s alc, propylene glycol
e160	Ethyl hexanoate	$CH_3(CH_2)_4CO_2C_2H_5$	144.21	2, 323	0.871^{20}_4	1.4075^{20}	−67	166–168	49	i aq; misc alc, eth
e161	2-Ethylhexanoic acid	$CH_3(CH_2)_3CH(C_2H_5)CO_2H$	144.21	2, 349	0.9077	1.4241^{20}	−118.4	228	127	0.25 aq
e162	2-Ethyl-1-hexanol	$CH_3(CH_2)_3CH(C_2H_5)CH_2OH$	130.23	Merck: 12, 3854	0.8319^{25}	1.4300^{20}	−70	184.6	73	0.07 aq; s alc, bz, chl
e163	2-Ethylhexanoyl chloride	$CH_3(CH_2)_3CH(C_2H_5)COCl$	162.66	2^2, 304	0.939	1.4335^{20}		68^{11mm}	69	
e164	2-Ethylhexyl acetate	$CH_3(CH_2)_3CH(C_2H_5)$-$CH_2O_2CCH_3$	172.27	Merck: 12, 6860	0.8718	1.4204^{20}	−80	199	71	0.03 aq; misc alc, oils, org liquids
e165	2-Ethylhexyl acrylate	$H_2C{=}CCO_2CH(C_2H_5)(CH_2)_3CH_3$	184.28	2^3, 1229	0.885	1.4358		214–219	79	
e166	2-Ethylhexylamine	$CH_3(CH_2)_3CH(C_2H_5)CH_2NH_2$	129.31	4^3, 388	0.789	1.4300^{20}	−76	169	60	i aq; s alc, acet, eth
e167	2-Ethylhexyl chloroformate	$CH_3(CH_2)_3CH(C_2H_5)CH_2O_2CCl$	192.69	3^4, 28	0.981	1.4312^{20}		107^{30mm}	81	
e168	2-Ethylhexyl cyanoacetate	$NCCH_2CO_2CH_2CH(C_2H_5)$-$(CH_2)_3CH_3$	197.28		0.975	1.4380^{20}		150^{11mm}	>110	
e169	2-Ethylhexyl 2-cyano-3,3-diphenylacrylate	$(C_6H_5)_2C{=}C(CN)CO_2CH_2$-$CH(C_2H_5)(CH_2)_3CH_3$	361.49		1.051	1.5670^{20}	−10	$218^{1.5mm}$	>110	

Ethylene glycol dimethyl ether, d505
Ethylene glycol ethyl ether acetate, e42
Ethylene glycol monoacetate, h120
Ethylene glycol monobutyl ether, b493
Ethylene glycol monobutyl ether acetate, b497
Ethylene glycol monoethyl ether, e40
Ethylene glycol monomethyl ether, m71
Ethylene glycol monomethyl ether acetate, m75
Ethylene iodide, d451
Ethylene iodohydrin, i32
1,8-Ethylenenaphthalene, a2
Ethylenethiourea, i4
Ethylene trichloride, t232
Ethyleneurea, i5
N-Ethylethanamine, d323
Ethyl 2-ethoxyglycolate, e149
Ethyl *N*-ethylcarbamate, e275
Ethyl fluoride, f17
2-Ethyl-1-hexanamine, e166
2-Ethylhexyl alcohol, e162



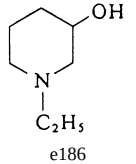
e155

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
e170	2-Ethylhexyl 4-(dimethylamino)-benzoate	$(CH_3)_2NC_6H_4CO_2CH_2$-$CH(C_2H_5)(CH_2)_3CH_3$	277.41		0.995	1.5420^{20}		325	>110	
e171	2-Ethylhexyl glycidyl ether	$CH_3(CH_2)_3CH(C_2H_5)CH_2$-$OCH_2CH(O)CH_2$	186.30		0.891	1.4340^{20}		$61^{0.3mm}$	96	
e172	2-Ethylhexyl methacrylate	$H_2C{=}C(CH_3)CO_2CH_2$-$CH(C_2H_5)(CH_2)_3CH_3$	198.31	2[3], 1289	0.885	1.4381^{20}		120^{18mm}	92	
e173	2-Ethylhexyl nitrate	$CH_3(CH_2)_3CH(C_2H_5)CH_2ONO_2$	175.23		0.963	1.4320^{20}			75	explodes when heated
e174	2-Ethylhexyl salicylate	2-$(HO)C_6H_4CO_2CH_2$-$CH(C_2H_5)(CH_2)_3CH_3$	250.34	10[3], 124	1.014	1.5020^{20}		190^{21mm}	>110	
e175	2-Ethylhexyl vinyl ether	$CH_3(CH_2)_3CH(C_2H_5)$-$CH_2OCH{=}CH_2$	156.26		0.8102	1.4273^{20}	−85	177–178	52	0.01 aq
e176	Ethyl hydrocinnamate	$C_6H_5CH_2CH_2CO_2C_2H_5$	178.23	9, 511	1.010	1.4940^{20}		247–248	107	
e177	Ethyl hydrogen hexanedioate	$HO_2C(CH_2)_4CO_2C_2H_5$	174.20	2[1], 277		1.4387^{20}	28–29	180^{18mm}	>110	
e178	Ethyl 4-hydroxybenzoate	$HOC_6H_4CO_2C_2H_5$	166.18	10, 159			116–118	297–298		0.07 aq; v s alc, eth
e179	Ethyl 3-hydroxybutyrate	$CH_3CH(OH)CH_2CO_2C_2H_5$	132.16	3, 309	1.017_4^{20}	1.4205^{20}		170	64	s aq, alc
e180	Ethyl 2-hydroxyethyl sulfide	$HOCH_2CH_2SCH_2CH_3$	106.19	1[2], 525	1.020	1.4869^{20}		180–184	>110	s eth
e181	Ethyl 6-hydroxyhexanoate	$HO(CH_2)_5CO_2C_2H_5$	160.22	3,3,628	0.985	1.4370^{20}		128^{12mm}	>110	
e182	Ethyl 2-hydroxyisobutyrate	$(CH_3)_2C(OH)CO_2C_2H_5$	132.16	3, 315	0.965	1.4078^{20}		150	44	dec by hot aq
e183	2-Ethyl-2-(hydroxymethyl)-1,3-propanediol	$C_2H_5C(CH_2OH)_3$	134.18	1[3], 2349			60–62	161^{2mm}		
e184	2-Ethyl-2-(hydroxymethyl)-1,3-propanedioltriacrylate	$(H_2C{=}CHCO_2CH_2)_3CC_2H_5$	296.32		1.100	1.4736^{20}		157	>110	

e185	2-Ethyl-2-(hydroxymethyl)-1,3-propanedioltrimethacrylate	$[H_2C{=}C(CH_3)CO_2CH_2]_3CC_2H_5$	338.40		1.060	1.4724^{20}			>110	
e186	*N*-Ethyl-3-hydroxypiperidine		129.20	Merck: 12, 3890	0.970	1.4754^{20}		95^{15mm}	47	
e187	2,2′-Ethylidenebis(4,6-di-*tert*-butylphenol)	$CH_3CH\{C_6H_2[C(CH_3)_3]_2OH\}_2$	438.70				162–164			
e188	2,2′-Ethylidenebis(4,6-di-*tert*-butylphenyl) fluorophosphite		486.66				201–203			
e189	4,4′-Ethylidenebisphenol	$CH_3CH_2CH(C_6H_4OH)_2$	214.26	6, 1006			123–127			
e190	5-Ethylidene-2-norborene		120.20		0.893	1.4895			38	
e191	2-Ethylimidazole		96.13	23, 78			86	268		
e192	Ethyl isobutyrate	$(CH_3)_2CHCO_2C_2H_5$	116.16	2, 291	0.870^{20}	1.3903^{20}	−88	110	13	misc alc, eth; sl s aq
e193	Ethyl isothiocyanate	CH_3CH_2NCS	87.14	4, 123	1.003^{18}_{4}	1.5142^{18}	−6	130–132	32	i aq; misc alc, eth

Ethyl hexyl ketone, n100
Ethyl hydrogen adipate, e177
N-Ethyl-*N*-(2-hydroxyethyl)-3-toluidine, e267
Ethyl 2-hydroxy-2-methylpropanoate, e182
Ethyl 2-hydroxypropionate, e194
Ethylidene bromide, d96
Ethylidene chloride, d225
Ethylidene dimethyl ether, d504
Ethylidene fluoride, d407
2,2′-Ethyliminodiethanol, e125
Ethyl iodide, i31
Ethyl isopentanoate, e208
Ethyl isonipicotate, e250
Ethyl isopropylactate, e208
Ethyl isothiocyanatoformate, e39
Ethyl isovalerate, e208



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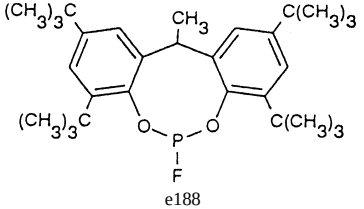

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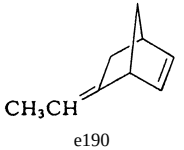

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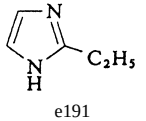


e191

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

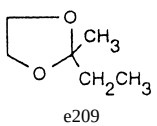
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
e194	Ethyl (−)-lactate	$CH_3CH(OH)CO_2C_2H_5$	118.13	3, 264	1.0328^{20}	1.4124^{20}	−26	154–155	46	misc aq, alc, eth, esters, PE
e195	Ethyl (±)-mandelate	$C_6H_5CH(OH)CO_2C_2H_5$	180.21	10, 202	1.115	1.5120^{20}	33–34	253–255	>110	
e196	Ethyl 2-mercaptoacetate	$HSCH_2CO_2C_2H_5$	120.17	3, 255	1.0964	1.4571^{20}		54^{12mm}	47	s alc, eth
e197	Ethyl 3-mercaptopropionate	$HSCH_2CH_2CO_2C_2H_5$	134.20	3^3, 555	1.039	1.4570^{20}		76^{10mm}	72	
e198	Ethylmercury chloride	CH_3CH_2HgCl	165.13		3.5		192	sublimes		0.78 eth; 2.6 chl
e199	Ethyl methacrylate	$H_2C{=}C(CH_3)CO_2C_2H_5$	114.14	2, 423	0.917	1.4116^{25}		118	15	i aq; s alc, eth
e200	Ethyl 4-methoxyphenylacetate	$CH_3OC_6H_4CO_2C_2H_5$	194.23	10^1, 83	1.097	1.5075^{20}		138^{7mm}	46	
e201	Ethyl 2-methylacetoacetate	$CH_3C(=O)CH(CH_3)CO_2C_2H_5$	144.17	3, 679	1.019	1.4280^{20}		187	62	i aq; s alc, eth
e202	*N*-Ethyl-2-methylallylamine	$H_2C{=}C(CH_3)CH_2NHC_2H_5$	99.18	4^4, 1104	0.753	1.4221^{20}		105	7	
e203	*N*-Ethyl-*N*-methylaniline	$C_6H_5N(CH_3)C_2H_5$	135.21	12, 162	0.947	1.5470^{20}		203–205	74	i aq; misc alc, eth
e204	Ethyl 2-methylbenzoate	$CH_3C_6H_4CO_2C_2H_5$	164.21	9, 463	1.032	1.5070^{20}		221^{731mm}	91	
e205	Ethyl 3-methylbenzoate	$CH_3C_6H_4CO_2C_2H_5$	164.21	9, 476	1.030	1.5054^{20}		110^{20mm}	101	
e206	Ethyl 4-methylbenzoate	$CH_3C_6H_4CO_2C_2H_5$	164.21	9, 484	1.025	1.5085^{20}		235	99	
e207	Ethyl 2-methylbutyrate	$CH_3CH_2CH(CH_3)CO_2C_2H_5$	130.19	2, 305	0.869	1.3969^{20}		133	26	
e208	Ethyl 3-methylbutyrate	$(CH_3)_2CHCH_2CO_2C_2H_5$	130.19	2^2, 275	0.8656^{20}	1.3962^{20}	−99	135	26	0.2 aq; misc alc, bz
e209	2-Ethyl-2-methyl-1,3-dioxolane		116.16	19^2, 11	0.929	1.4090^{20}		116–117	12	
e210	Ethyl methyl ether	$C_2H_5OCH_3$	60.10	1, 314	2.456 g/L		−113	7.4		s aq; misc alc, eth

e210a	3-Ethyl-4-methyl-hexane	$(C_2H_5)_2CHCH(CH_3)C_2H_5$	128.26		0.7420^{20}	1.4134^{20}		140	24	
e211	2-Ethyl-4-methyl-imidazole		110.16	23^{2}, 72	0.975	1.5000^{20}	47–54	292–295	137	
e212	Ethyl 4-methyl-5-imidazolecarboxylate		154.17	25^{1}, 534			204–206			
e213	4-Ethyl-2-methyl-2-(3-methylbutyl)-oxazolidine		185.3		0.877	1.4420^{20}		194	82	
e214	3-Ethyl-2-methyl-pentane	$(C_2H_5)_2CHCH(CH_3)_2$	114.24	1^{3}, 489	0.7193_4^{20}	1.4040^{20}	−115.0	115.7	<21	i aq; sl s alc; s eth
e215	3-Ethyl-3-methyl-pentane	$(C_2H_5)_3CCH_3$	114.24		0.7274^{20}	1.4078^{20}	−90.9	118.3		i aq; s eth
e216	Ethyl 1-methyl-2-piperidinecarboxylate		171.24	22^{1}, 485	0.975	1.4519^{20}		96^{11mm}	73	
e217	Ethyl 1-methyl-3-piperidinecarboxylate		171.24		0.954	1.4510^{20}		89^{11mm}	68	

Ethyl levulinate, e236
Ethyl linoleate, e229
Ethyl mercaptan, e26a

Ethyl 3-methylcrotonate, e126
Ethyl methyl ketone, b475
Ethyl 1-methylnipecotate, e216

Ethyl 2-methyl-4-oxo-2-cyclohexene-1-carboxylate, c7
Ethyl *N*-methyl-*N*-phenylcarbamate, m379
Ethyl 2-methylpipicolinate, e217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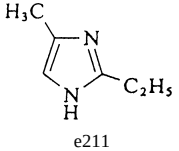
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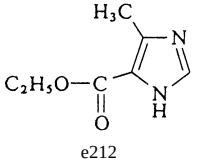
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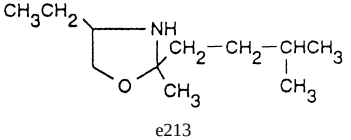
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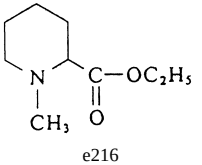
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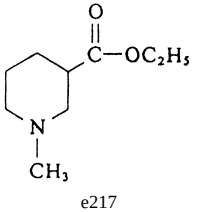
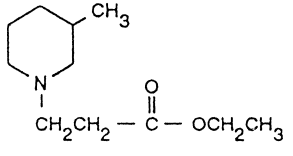

e217

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
e218	Ethyl 3-methyl-1-piperidine propionate		199.30	2^{2}, 59	0.945	1.4530^{20}		112^{13mm}	99	
e219	2-Ethyl-2-methyl-1,3-propanediol	$HOCH_2C(C_2H_5)(CH_3)CH_2OH$	118.18	1, 487			41–44	226	>110	
e220	5-Ethyl-2-methylpyridine	$C_2H_5(CH_3)C_5H_3N$	121.18	20, 248	0.919	1.4970^{20}		178	66	s alc, bz, eth, acid
e221	Ethyl methyl sulfide	$CH_3CH_2SCH_3$	76.15	1, 343	0.842	1.4392^{20}	−106	66.7	−15	i aq; misc alc, eth
e222	Ethyl (methylthio)-acetate	$CH_3SCH_2CO_2C_2H_5$	134.20		1.043	1.4587^{20}		72^{25mm}	59	
e223	*N*-Ethylmorpholine		115.18	27^{1}, 203	0.905	1.4410^{20}	−63	139	27	misc aq, alc, eth
e224	Ethyl nitrate	$CH_3CH_2ONO_2$	91.13	1, 329	1.100_4^{25}	1.3849^{22}	−94.6	87.7	10 (CC)	1 aq; misc alc, eth
e225	Ethyl nitrite	CH_3CH_2ONO	75.07	1, 329	0.90_{15}^{15}			17	−35	misc alc, eth
e226	4-Ethylnitrobenzene	$C_2H_5C_6H_4NO_2$	151.17	5, 358	1.118	1.5445^{20}	−32	245–246	>110	v s alc, eth
e227	Ethyl 4-nitrobenzoate	$O_2NC_6H_4CO_2C_2H_5$	195.17	9, 390			55–59			
e228	Ethyl nonanoate	$CH_3(CH_2)_7CO_2C_2H_5$	186.30	2, 353	0.866	1.4219^{20}	−37	227	94	i aq; misc alc, eth
e229	Ethyl *cis*,*cis*-9,12-octadecadienoic acid	$H(CH_2)_5CH{=}CHCH_2CH{=}CH(CH_2)_7CO_2C_2H_5$	308.51	2^{2}, 461	0.8846	1.4675^{20}		193^{6mm}	>110	misc DMF, oils
e230	Ethyl *cis*-9-octadecenoate	$CH_3(CH_2)_7CH{=}CH(CH_2)_7CO_2C_2H_5$	310.53	2, 467	0.869	1.4500^{20}	−32	216^{15mm}	>110	i aq; misc alc, eth
e231	Ethyl octanoate	$CH_3(CH_2)_7CO_2C_2H_5$	172.27	2, 348	0.878	1.4166	−43	208	75	i aq; misc alc, eth
e232	Ethyl oxalyl chloride	$CH_3CH_2OC(=O)C(=O)Cl$	136.53	2, 541	1.2223	1.4164^{20}		135	41	d aq, alc; s bz, eth
e233	Ethyl oxamate	$CH_3CH_2OC(=O)C(=O)NH_2$	117.10	2, 544			114–116			s aq, eth; i bz
e234	2-Ethyl-2-oxazoline		99.13		0.982	1.4370^{20}	−62	128	29	
e235	Ethyl 2-oxocyclopentanecarboxylate	$(O{=})(C_5H_7)CO_2C_2H_5$	156.18	10, 597	1.054	1.4485^{20}		102^{11mm}	77	
e236	Ethyl 4-oxopentanoate	$CH_3C(=O)CH_2CH_2CO_2C_2H_5$	144.17	3, 675	1.012	1.4222^{20}		205–206		v s aq; misc alc
e237	Ethyl 2-oxopropionate	$CH_3C(=O)CO_2C_2H_5$	116.12	3, 616	1.060_4^{16}	1.408^{16}		144	45	sl s aq; misc alc, eth
e238	3-Ethylpentane	$(C_2H_5)_3CH$	100.20	1^{3}, 441	0.6982_4^{20}	1.3934^{20}	−118.6	93.5		i aq; s alc, eth
e239	Ethyl pentanoate	$CH_3(CH_2)_3CO_2C_2H_5$	130.19	2, 301	0.877_4^{20}	1.3732^{20}	−91.3	145.5		0.2 aq; misc alc, eth
e240	2-Ethylphenol	$C_2H_5C_6H_4OH$	122.17	5, 470	1.037	1.5372^{20}	−18	204	78	
e241	3-Ethylphenol	$C_2H_5C_6H_4OH$	122.17	6, 471	1.001	1.5330^{20}	−4	110^{15mm}	94	
e242	4-Ethylphenol	$C_2H_5C_6H_4OH$	122.17	6, 472	1.011	1.5239	45	218	100	i aq; misc alc, eth
e243	Ethyl phenylacetate	$C_6H_5CH_2CO_2C_2H_5$	164.20	9, 434	1.031	1.4980^{20}		229	77	i aq; misc alc, eth

e244	Ethyl 3-phenyl-glycidate		192.21		1.102	1.5180^{20}		$96^{0.5mm}$	>110	
e245	1-Ethylpiperazine		114.19	23^{2}, 5	0.899	1.4690^{20}		157	43	
e246	Ethyl *N*-piperazino-carboxylate		158.20	23^{2}, 9	1.080	1.4765^{20}		273	>110	
e247	1-Ethylpiperidine		113.20	20, 17	0.834	1.4440^{20}		131	18	
e248	2-Ethylpiperidine		113.20	20, 104	0.858	1.4510^{20}		143	31	s aq
e249	Ethyl 3-piperidine-carboxylate		157.21		1.012	1.4601^{20}		104^{7mm}	90	
e250	Ethyl 4-piperidine-carboxylate		157.21		1.010	1.4591^{20}		204	80	s aq, alc, bz, eth
e251	Ethyl *N*-piperidine-propionate		185.27	20, 62	0.927	1.4545^{20}		217–219	87	

Ethyl nipecotate, e249
Ethyl oleate, e230
Ethyl oxirane, e3
Ethyl pelargonate, e228
Ethyl pentyl ketone, o37
Ethyl phenyl ether, e36
Ethyl picolinate, e259
Ethylpiperidinol, e186
Ethyl pivalate, e128



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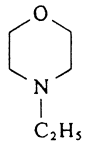

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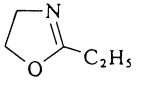

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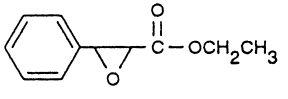

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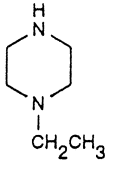

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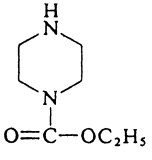

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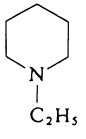

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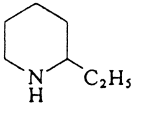

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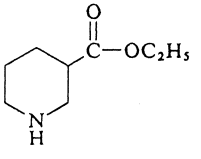

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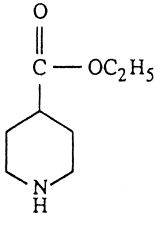

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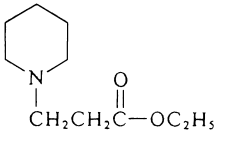

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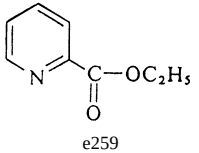
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
e252	Ethyl 1-propenyl ether	$CH_3CH{=}CHOC_2H_5$	86.13	1, 435	0.778	1.3980^{20}		67–76	−18	
e253	Ethyl propionate	$CH_3CH_2CO_2C_2H_5$	102.13	2, 240	0.8917^{20}	1.3839^{20}	−73.9	99	12	1.7 aq; misc alc, eth
e254	Ethyl propyl ether	$CH_3CH_2OCH_2CH_2CH_3$	88.15	1, 354	0.739	1.3695^{20}	−79	62–63	32	sl s aq; misc alc, eth
e255	Ethyl propyl sulfide	$CH_3CH_2SCH_2CH_2CH_3$	104.21	1[3], 1432	0.8270	1.4462^{20}	−117.0	118.5		s alc
e256	2-Ethylpyridine	$CH_3CH_2(C_5H_4N)$	107.16	20, 241	0.937	1.4964^{20}		149	29	sl s aq; s alc, eth
e257	3-Ethylpyridine	$CH_3CH_2(C_5H_4N)$	107.16	20, 242	0.954	1.5015^{20}		162–165	48	v s alc, eth; sl s aq
e258	4-Ethylpyridine	$CH_3CH_2(C_5H_4N)$	107.16	20, 243	0.942	1.5009^{20}		168	47	sl s aq; s alc, eth
e259	Ethyl 2-pyridine-carboxylate		151.17	22, 35	1.1194	1.5088^{20}	2	240–241	107	misc aq, alc, eth
e260	1-Ethyl-2-pyrrolidinone		113.16		0.992	1.4652^{20}		97^{20mm}	76	
e261	Ethyl salicylate	$C_6H_4(OH)CO_2C_2H_5$	166.18	10, 73	1.131	1.5219^{20}	2–3	232–234	107	misc alc, eth; sl s aq
e262	Ethyl sorbate	$CH_3CH{=}CHCH{=}CHCO_2C_2H_5$	140.18	2, 484	0.956	1.4942^{20}		195.5	69	
e262a	2-Ethyltoluene	$CH_3C_6H_4C_2H_5$	120.19	5[1], 192	0.865	1.5040^{20}	−81	165	39	
e262b	3-Ethyltoluene	$CH_3C_6H_4C_2H_5$	120.19	5, 398	0.865	1.4960^{20}	−95	161	38	
e262c	4-Ethyltoluene	$CH_3C_6H_4C_2H_5$	120.19	5, 397	0.861	1.4950^{20}	−62	162	36	
e263	Ethyl 4-toluene-sulfonate	$CH_3C_6H_4SO_2OC_2H_5$	200.26	11, 99	1.166_4^{45}	1.5110^{20}	33	173^{15mm}	157	i aq; s alc, eth
e264	*N*-Ethyl-*m*-toluidine	$CH_3C_6H_4NHC_2H_5$	135.21	12, 857	0.957	1.5451^{20}		221	89	
e265	*N*-Ethyl-*o*-toluidine	$CH_3C_6H_4NHC_2H_5$	135.21		0.938	1.5470^{20}		218	88	
e266	6-Ethyl-*o*-toluidine	$C_2H_5C_6H_3(CH_3)NH_2$	135.21		0.968	1.5525^{20}	−33	231	89	
e267	2-(*N*-Ethyl-*m*-toluidino)ethanol	$CH_3C_6H_4N(C_2H_5)CH_2CH_2OH$	179.26		1.019	1.5540^{20}		115^{1mm}	>110	
e268	Ethyl trichloroacetate	$Cl_3CCO_2C_2H_5$	191.44	2, 209	1.383_4^{20}	1.4447^{20}		168	65	i aq; s alc, eth
e269	Ethyltrichlorosilane	$C_2H_5SiCl_3$	163.51	4, 630	1.238	1.4252^{20}	−106	99	13	
e270	Ethyltriethoxysilane	$C_2H_5Si(OC_2H_5)_3$	192.33	4[4], 4223	0.895	1.3920^{20}		158–166	38	
e271	Ethyltriphenyl-phosphonium iodide	$C_2H_5P(C_6H_5)_3I$	418.26	16, 760			169–171			
e272	Ethyl undecanoate	$CH_3(CH_2)_{10}CO_2C_2H_5$	214.35	2, 358	0.859	1.4280^{20}		105^{4mm}	>110	i aq; s org solvents
e273	Ethyl 10-undecenoate	$H_2C{=}CH(CH_2)_8CO_2C_2H_5$	212.34	2, 459	0.879	1.4390^{20}		258–259	>110	
e274	Ethylurea	$CH_3CH_2NHC(=O)NH_2$	88.11	4, 115	1.213^{18}		93–96			v s aq; 80 alc; i eth
e275	*N*-Ethylurethane	$CH_3CH_2NHCO_2C_2H_5$	117.15	4, 114	0.981_4^{20}	1.4211^{20}		85^{20mm}	75	63 aq

e276	Ethyl vinyl ether	$CH_3CH_2OCH{=}CH_2$	72.11	1, 433	0.7589^{20}	1.3767^{20}	−116	35	< −45	0.9 aq; s alc, eth
e277	*N*-Ethyl-2,3-xylidine	$(CH_3)_2C_6H_3NHC_2H_5$	149.24	12, 1101	0.917	1.5468^{20}		228	71	
e278	1-Ethynyl-1-cyclohexanol	$HOC_6H_{10}C{\equiv}CH$	124.18	6[2], 100	0.967		31–33	180	62	2.4 aq; misc alc, bz, acet, ketones, PE
e279	Eugenol	4-$(H_2C{=}CHCH_2)C_6H_3$-2-$(OCH_3)OH$	164.20	6, 961	1.066	1.5410^{20}	−12/−10	254	>110	
f1	Fluoranthene		202.26	5, 685	1.252_4^0		108	384		sl s alc; s bz, eth
f2	Fluorene		166.22	5, 625	1.203_4^0		115	295		v s HOAc; s bz, eth
f3	Fluorenone		180.21	7, 465	1.1300_4^{99}	1.6369^{99}	82–85	342		s alc, bz; v s eth
f4	Fluorescein		332.31	19, 222			320			s hot alc, hot HOAc
f5	Fluoroacetic acid	FCH_2CO_2H	78.04	2, 193			33	165		sl s aq, alc
f6	4-Fluoroacetophenone	$FC_6H_4COCH_3$	138.14		1.138	1.5110^{20}		196	71	
f7	2-Fluoroaniline	$FC_6H_4NH_2$	111.12	12[1], 296	1.151	1.5420^{20}	−29	183	60	
f8	4-Fluoroaniline	$FC_6H_4NH_2$	111.12	12, 597	1.1725	1.5395^{20}	−2	187	73	sl s aq; s alc, eth
f9	2-Fluorobenzaldehyde	FC_6H_4CHO	124.11	7[1], 132	1.178	1.5220^{20}	−44.5	91^{46mm}	55	
f10	4-Fluorobenzaldehyde	FC_6H_4CHO	124.11	7[1], 132	1.157	1.5200^{20}	−10	181	56	
f11	Fluorobenzene	C_6H_5F	96.11	5, 198	1.0240_4^{20}	1.4657^{20}	−42.2	84.7	−15	0.15 aq; misc alc
f12	2-Fluorobenzoic acid	$FC_6H_5CO_2H$	140.11	9, 333	1.460_4^{25}		123–125			sl s aq; s alc, eth
f13	4-Fluorobenzoic acid	$FC_6H_5CO_2H$	140.11	9, 333	1.479_4^{25}		184–187			0.1 aq; s alc, eth

1-Ethyl-1-propanol, p41
Ethyl propenoate, e60
1-Ethylpropylamine, a247a
Ethyl pyruvate, e237
2-(Ethylthio)ethanol, e180
Ethyl thioglycolate, e196
Ethyl toluates, e204, e205, e206
Ethyl *p*-tolyl ether, m373
Ethyl trimethylacetate, e128
Ethyl vanillin, e46
Ethyne, a41
Ethynylbenzene, p84
Eugenol, m108
Eugenol methyl ether, a84
Fenchone, t376
Fenchyl alcohol, t375
N-9*H*-(2-Fluorenyl)acetamide, a13



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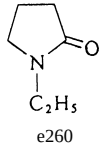

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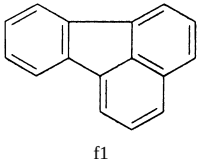
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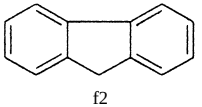
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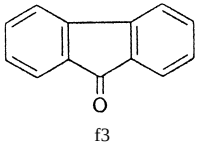

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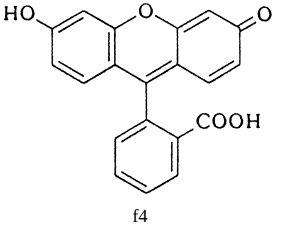

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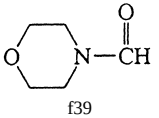
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
f14	2-Fluorobenzoyl chloride	FC_6H_5COCl	158.56	9^{1}, 136	1.328	1.5365^{20}	4	92^{15mm}	82	
f15	4-Fluorobenzoyl chloride	FC_6H_5COCl	158.56	9^{1}, 137	1.342	1.5296^{20}	9	82^{20mm}	82	
f16	4-Fluorobenzyl chloride	$FC_6H_5CH_2Cl$	144.58		1.207	1.5130^{20}		82^{26mm}	60	
f17	Fluoroethane	CH_3CH_2F	48.06	1, 82			−143.2	−37.7		198 mL aq; v s alc, eth
f18	Fluoromethane	CH_3F	34.04	1, 59	1.195 g/L		−141.8	−78.4		166 mL aq; v s alc, eth
f19	3-Fluoro-1-methoxy-benzene	$FC_6H_4OCH_3$	126.13		1.104	1.4880^{20}		158^{743mm}	43	
f20	4-Fluoro-1-methoxy-benzene	$FC_6H_4OCH_3$	126.13	6^{1}, 98	1.114	1.4877^{20}	−45	157	43	s eth
f21	2-Fluoro-2-methyl-propane	$(CH_3)_3CF$	76.11	1^{4}, 286			−77	12	−12	
f22	4-Fluoro-3-nitroaniline	$FC_6H_3(NO_2)NH_2$	156.12	12, 729			96–98		91	
f23	1-Fluoro-4-nitro-benzene	$FC_6H_4NO_2$	141.10	5, 241	1.3300_4^{20}	1.5312^{20}	21	205	83	i aq; s alc, eth
f24	4-Fluoro-3-nitro-toluene	$CH_3C_6H_3(NO_2)F$	155.13		1.262	1.5240^{20}	28–30	241	>110	
f25	4-Fluorophenol	FC_6H_4OH	112.10	6, 183			46–48	185	68	
f26	2-Fluoropyridine	$F(C_5H_4N)$	97.09	20^{1}, 80	1.128	1.4680^{20}		126	28	
f27	2-Fluorotoluene	$FC_6H_4CH_3$	110.13	5, 290	1.0014^{17}	1.4716^{17}	−62	115	12	v s alc, eth
f28	3-Fluorotoluene	$FC_6H_4CH_3$	110.13	5, 290	0.9974^{20}	1.4691^{20}	−87	115	9	s alc, eth
f29	4-Fluorotoluene	$FC_6H_4CH_3$	110.13	5, 290	0.9975^{20}	1.4698^{20}	−56	117	17	s alc, eth
f30	Fluorotrichloro-methane	$FCCl_3$	137.37	1, 64	1.494	1.3821^{20}	−110	24	none	
f31	Formaldehyde	$H_2C{=}O$	30.03	1, 558	0.815^{-20}_{4}	0.8153^{-20}	−92	−19.5	56	122 aq; s alc, eth
f32	Formamide	$HC(=O)NH_2$	45.04	2, 26	1.1334_4^{20}	1.4475^{20}	2.6	220	154	misc aq, alc, acet
f33	Formamidine acetate	$HC(=NH)NH_2 \cdot HO_2CCH_3$	104.11				158 dec			
f34	Formamidinesulfinic acid	$H_2NC(=NH)S(O)OH$	108.12	3^{1}, 36			126 dec			
f35	Formanilide	C_6H_5NHCHO	121.14	12, 230	1.144		47	271	>110	2.5 aq
f36	Formic acid	HCO_2H	46.03	2, 8	1.220_4^{20}	1.3704^{20}	8.3	100.8	68	misc aq, alc, eth
f37	2-Formylbenzoic acid	$HO_2CC_6H_4HCO$	150.13	10, 666	1.404		96–98			s aq; v s alc, eth

f38	Formylhydrazine	$HC(=O)NHNH_2$	60.06	2, 93			54–56		>110	v s alc, chl, eth; s bz
f39	4-Formylmorpholine		115.13	27^3, 274	1.145	1.4848^{20}		236–237	>110	
f40	*N*-Formylpiperidine		113.16	20, 45	1.019	1.4780^{20}		222	91	
f41	**D**-(−)-Fructose		180.16	31, 321				122 dec		v s aq; 6.7 alc; s pyr
f42	Fumaric acid	$HO_2CCH{=}CHCO_2H$	116.07	2, 737	1.635_4^{20}		287	subl 300		0.6 aq; 9 alc; 0.7 eth
f43	Fumaroyl dichloride	$ClC(=O)CH{=}CHC(=O)Cl$	152.96	2, 743	1.408^{20}	1.4988^{20}		161–164	73	dec aq, alc
f44	2-Furaldehyde		96.09	17^2, 305	1.1598_4^{20}	1.5262^{20}	−36.5	161.8	60	8 aq; misc alc, eth
f45	Furan		68.07	17, 27	0.9514^{20}	1.4214^{20}	−85.6	31.4	−35	1 aq; misc alc, eth
f46	2-Furanacrylic acid		138.12	18, 300			142–144	286		0.2 aq; 1.1 bz; s alc, eth, HOAc
f47	2,5-Furandimethanol		128.13	17^1, 90			74–76			
f48	2-Furanmethanethiol		114.17	17^2, 116	1.132	1.5304^{20}		155	45	

Fluorothane, b308
Fluorotrichloromethane, t237
2-Fluoro-5-(trifluoromethyl)aniline, a179
Formal, d507
Formaldehyde diethyl acetal, d307
Formic acid hydrazide, f38
Formylamide, f33
Formylphenols, h94, h95, h96
Formylpyridines, p261, p262, p263
Freon-11, t237
Freon-12, d218
Freon-12B2, d93
Freon-21, d233
Freon-22, c101
Freon-114, d271
2,5-Furandione, m2
2-Furanmethanol, f50
Furfural, f44
2-Furfuraldehyde, f44



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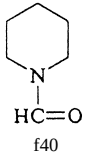

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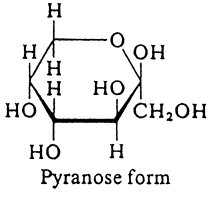

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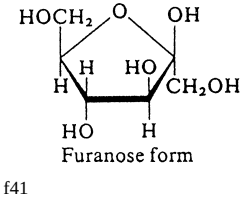

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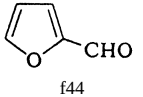

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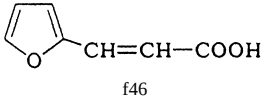

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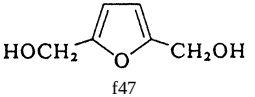

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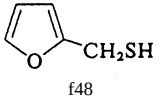

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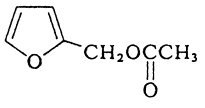
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
f49	Furfuryl acetate		140.14	17^{2}, 115	1.1175_{4}^{20}	1.4618^{20}		175–177	65	i aq; s alc, eth
f50	Furfuryl alcohol		98.10	17, 112	1.1295_{4}^{20}	1.4868^{20}	−31	171	75	misc aq(dec); v s alc, eth
f51	Furfurylamine		97.12	18, 584	1.0995_{4}^{20}	1.4900^{20}	−70	145–146	46	misc aq; s alc, eth
f52	Furfuryl methacrylate		166.18	17^{3}, 1248	1.078	1.4820^{20}		82^{5mm}	90	
f53	α-Furildioxime		220.18	19, 166			166–168			v s alc, eth; sl s bz
f54	2-Furoic acid		112.08	18, 272			133–134	230–232		4 aq; s alc; v s eth
f55	2-Furoyl chloride		130.53	18, 276	1.324	1.5310^{20}	−2	170	85	dec aq, alc; s eth
g1	**D**-(+)-Galactose		180.16	31, 295			167			200 aq; s pyr; sl s alc
g2	Geraniol	$(CH_3)_2C{=}CHCH_2CH_2$-$C(CH_3){=}CHCH_2OH$	154.25	1, 457	0.8894_{4}^{20}	1.4766^{20}		230	76	i aq; misc alc, eth
g3	Geranyl acetate	$(CH_3)_2C{=}CHCH_2CH_2$-$C(CH_3){=}CHCH_2O_2CCH_3$	196.29	2, 140	0.9174_{15}^{15}	1.4628^{15}		138^{25mm}	104	v s alc; misc eth
g4	Gerard reagent P	$[(C_5H_5N)CH_2C(=O)NHNH_2]^+ Cl^-$	187.63	Merck: 12, 4436			dec 200			less soluble in polar solvents than T
g5	Gerard reagent T	$[(CH_3)_3NCH_2C(=O)NHNH_2]^+ Cl^-$	167.64	Merck: 12, 4436			192			v s aq, HOAc, glyc, ethylene glycol
g6	**D**-Gluconic acid		196.16	3, 542			131			v s aq; sl s alc; i eth
g7	δ-Gluconolactone		178.14	18^{1}, 405			153			50 aq; 1 alc; i eth
g8	α-**D**-(+)-Glucose		180.16	31, 83	1.5620_{4}^{18}		153–156			91 aq; 0.83 MeOH; s pyr
g9	α-**D**-Glucose penta-acetate		390.34	31, 119			109–111			0.15 aq; 1.3 alc; 3 eth
g11	**D**-Glucurono-3,6-lactone		176.12	Merck: 11, 4362			176–178			27 aq; 2.8 MeOH
g12	(*S*)-(+)-Glutamic acid	$HO_2CCH_2CH_2CH(NH_2)CO_2H$	147.13	4, 488	1.538_{4}^{20}		d 247	subl 200		0.8 aq; i alc, eth
g13	(*S*)-(+)-Glutamine	$H_2NC(=O)CH_2CH_2$-$CH(NH_2)CO_2H$	146.15	4, 491			185 dec			5 aq; 0.0035 MeOH; i bz, chl, eth, acet
g14	Glutaric acid	$HO_2CCH_2CH_2CH_2CO_2H$	132.12	2, 631	1.429_{4}^{20}	1.4188^{106}	98	303		43 aq^{20}; v s alc, eth; s bz, chl; sl s PE
g15	Glutaric anhydride		114.10	17, 411			55–57	150^{10mm}	>110	
g16	Glutaric dialdehyde	$OCHCH_2CH_2CH_2CHO$	100.12	1, 776		1.4338^{25}		187–189	none	s aq, alc
g17	Glutaronitrile	$NCCH_2CH_2CH_2CN$	94.12	2, 635	0.9888^{23}	1.4345^{20}	−29	286	>110	s aq, alc, chl; i eth

g18	Glutaryl dichloride	$ClC(=O)(CH_2)_3C(=O)Cl$	169.01	2, 634	1.324	1.4720^{20}		216–218	106	dec aq, alc; s eth
g19	Glycerol	$HOCH_2CH(OH)CH_2OH$	92.09	1, 502	1.2613^{20}	1.4746^{20}	18	290	199	misc aq, alc; 0.2 eth
g20	Glyceryl tris(butyrate)	$(CH_3CH_2CH_2CO_2CH_2)_2CH$-$O_2CCH_2CH_2CH_3$	302.37	2, 273	1.032_4^{20}	1.4359^{20}	−75	287–288	173	i aq; v s alc, eth

Furfuryl mercaptan, f48
Furylacrylic acid, d46
2-Furyl methyl ketone, a44
Galactitol, d824
Gallic acid, t319
Gentisic acid, d432
Geranial, d665
D-Glucitol, s5
Glutaraldehyde, g16
Glycerol dichlorohydrin, d264
Glycerol α-monochlorohydrin, c227
Glyceryl triacetate, p200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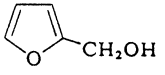
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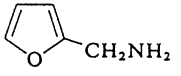
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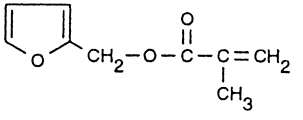
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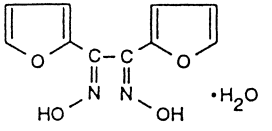
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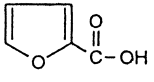
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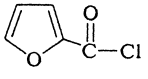
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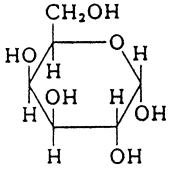
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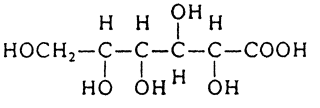
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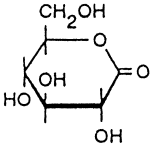
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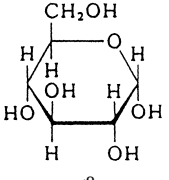
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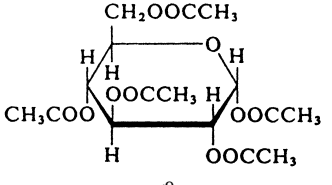
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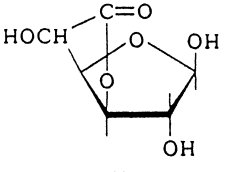
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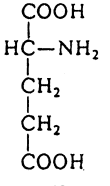
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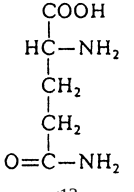
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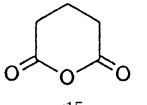
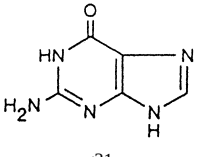

g15

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
g21	Glyceryl tris-(dodecanoate)	$[CH_3(CH_2)_{10}CO_2CH_2]_2CH$-$O_2C(CH_2)_{10}CH_3$	639.02	2, 362	0.894_4^{60}	1.4404^{60}	46			v s bz, eth; sl s alc
g22	Glyceryl tris(nitrate)	$O_2NOCH_2CH(ONO_2)CH_2ONO_2$	227.09	1, 516	1.594_4^{20}	1.4786^{12}	13.3	160^{5mm}	explodes 270	0.18 aq; 54 alc; misc eth
g23	Glyceryl tris(oleate)	$[CH_3(CH_2)_7CH{=}CH(CH_2)_7$-$CO_2CH_2]_2CHO_2C(CH_2)_7$-$CH{=}CH(CH_2)_7CH_3$	885.46	4, 468	0.915_4^{15}	1.4621^{40}	−4/−5	235^{15mm}		s chl, eth, CCl_4
g24	Glyceryl tris(palmitate)	$[CH_3(CH_2)_{14}CO_2CH_2]_2CH$-$O_2C(CH_2)_{14}CH_3$	807.35	2, 373	0.8663_4^{80}	1.4381^{80}	65–66	310–320		v s bz, chl, eth
g25	Glyceryl tris-(tridecanoate)	$[CH_3(CH_2)_{11}CO_2CH_2]_2CH$-$O_2C(CH_2)_{11}CH_3$	723.18	2, 367	0.885_4^{60}	1.4428^{60}	57			v s alc, bz, chl
g26	Glycine	$H_2NCH_2CO_2H$	75.07	4, 333	1.1607		dec 240			25 aq; 0.6 pyr; i eth
g27	*N*-Glycylglycine	$H_2NCH_2C(=O)NHCH_2CO_2H$	132.12	4, 371			260 dec			s hot aq; sl s alc
g28	Glyoxal	$HC(=O)CHO$	58.04	1, 759	1.14	1.3826^{20}	15	50.4		viol rxn aq; s anhyd solvents; mixtures with air may explode
g29	Glyoxylic acid	$HC(=O)CO_2H$	74.04	3, 594			98			v s aq; sl s alc, eth
g30	Guanidine	$H_2NC(=NH)NH_2$	59.07	3, 82			*ca.* 50	dec 160		v s aq, alc
g31	Guanine		151.13	26, 449			>300			s alk soln, dil acids; sl s alc, eth
h1	Heptadecane	$CH_3(CH_2)_{15}CH_3$	140.41	1, 173	0.7767^{22}	1.4360^{25}	22.0	302.2	148	s eth; sl s alc
h1a	1-Heptadecanol	$CH_3(CH_2)_{16}OH$	256.48	1[1], 220			53.8	333	>110	
h2	Heptafluorobutyric acid	$CF_3CF_2CF_2CO_2H$	214.04		1.625	$<1.300^{20}$		120	none	
h3	Heptaldehyde	$CH_3(CH_2)_5CHO$	114.19	1[2], 750	0.8216_4^{15}	1.4285^{20}	−43	153	35	misc alc, eth; sl s aq
h4	2,2,4,4,6,8,8-Hepta-methylnonane	$(CH_3)_3CCH_2C(CH_3)_2CH_2$-$CH(CH_3)CH_2C(CH_3)_3$	226.45		0.793	1.4391^{20}		240	95	
h5	1,1,1,3,5,5,5-Hepta-methyltrisiloxane	$[(CH_3)_3SiO]_2SiHCH_3$	222.51	4[3], 1874	0.819	1.3820^{20}		142	27	
h6	Heptane	$CH_3(CH_2)_5CH_3$	100.21	1, 154	0.6838_4^{20}	1.3877^{20}	−90.6	98.4	−4 (CC)	s alc, chl, eth
h7	Heptanedioic acid	$HO_2C(CH_2)_5CO_2H$	160.17	2, 670	1.329^{15}		105.8	212^{10mm}		5 aq; v s alc, eth
h8	1-Heptanethiol	$CH_3(CH_2)_6SH$	132.27	1, 415			−43.2	176.9	46	i aq

h9	Heptanoic acid	$CH_3(CH_2)_5CO_2H$	130.19	2, 338	0.9181_4^{20}	1.4221^{20}	−8	222	>110	0.25 aq; s alc, eth
h10	Heptanoic anhydride	$[CH_3(CH_2)_5CO]_2O$	242.36	2, 340	0.923	1.4332^{20}	−12.4	268	>110	i aq; s alc, eth
h11	1-Heptanol	$CH_3(CH_2)_6OH$	116.20	1, 414	0.8219_4^{20}	1.4242^{20}	−34	176.4	73	misc alc, eth
h12	2-Heptanol	$CH_3(CH_2)_5CH(OH)CH_3$	116.20	1, 415	0.8167^{20}	1.4210^{10}		159	71	0.35 aq; s alc, bz, eth
h13	3-Heptanol	$CH_3(CH_2)_3CH(OH)CH_2CH_3$	116.20	1[1], 205	0.8227^{20}	1.4214^{20}	−70	157	60	sl s aq
h14	2-Heptanone	$HC_3(CH_2)_4C(=O)CH_3$	114.19	1, 699	0.8197_4^{15}	1.4116^{15}	−35	151	39	s alc, eth
h15	3-Heptanone	$CH_3(CH_2)_3C(=O)CH_2CH_3$	114.19	1, 699	0.8197_{20}^{20}	1.4055^{20}	−39	147	46	0.43 aq; s alc, eth
h16	4-Heptanone	$CH_3(CH_2)_2C(=O)(CH_2)_2CH_3$	114.19	1, 699	0.817	1.4068^{20}	−32.1	143.7	48 (CC)	0.53 aq; misc alc, eth
h17	Heptanoyl chloride	$CH_3(CH_2)_5C(=O)Cl$	148.63	2, 340	0.960	1.4300^{20}		173	58	dec aq, alc; s eth
h18	1-Heptene	$CH_3(CH_2)_4CH=CH_2$	98.90	1, 219	0.6970^{20}	1.3999^{20}	−120	93.6	−8	0.1 aq; s alc, eth
h18a	*cis*-2-Heptene	$CH_3(CH_2)_3CH=CHCH_3$	98.19	1[3], 825	0.708^{20}	1.406^{20}		98.4	−6	
h18b	*trans*-2-Heptene	$CH_3(CH_2)_3CH=CHCH_3$	98.19	1, 219	0.7012^{20}	1.4045^{20}	−109.5	98	−1	
h19	1-Heptylamine	$CH_3(CH_2)_6NH_2$	115.22	4, 193	0.777	1.4243^{20}	−23	154–56	35	s alc, acet, eth, PE
h20	1-Heptyne	$CH_3(CH_2)_4C\equiv CH$	96.17	1, 256	0.733	1.4075^{20}	−81	99–100	−2	
h21	Hexachloroacetone	$Cl_3CC(=O)CCl_3$	264.75	1, 657	1.743	1.5112^{20}	−30	66^{6mm}	none	sl s aq; s acet
h22	Hexachlorobenzene	CCl_6	284.78	5, 205	2.044^{24}		232	325	242	s bz, chl, eth
h23	Hexachloro-1,3-butadiene	$CL_2C=CClCCl=CCl_2$	260.76	1, 250	1.655	1.5550^{20}	−21	215	none	s alc, eth
h24	1,2,3,4,5,6-Hexachloro-cyclohexane, γ-isomer	$C_6H_6Cl_6$	290.83	5[1], 8	1.87^{20}		113–115			s bz, chl

Glyceryl tris(laurate), g21
Glyceryl tris(myristate), g25
Glycidic acid, h88
Glycidol, e16
Glycidyl methacrylate, e17
Glycidyl phenyl ether, e14
Glycinol, e29
Glycinonitrile, a103
Glycolaldehyde, h87
Glycolaldehyde diethyl acetal, d305
Glycolic acid, h88
Glycol methacrylate, h126
Glyoxaline, i3
Guaiacol, m97
Heliotropin, m250
Hemimellitene, t357
Hemimellitic acid, b29
Heptaldehyde, h3
sec-Heptyl alcohol, h12
Heptyl bromide, b343
Heptyl chloride c147
Heptyl iodide, i34
Heptyl mercaptan, h8
Heptyl methyl ketone, n99



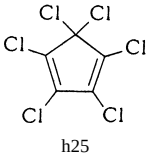
g31

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
h25	Hexachlorocyclo-1,3-pentadiene		272.77		1.701_4^{25}	1.5644^{20}	−10	239	none	
h27	Hexachloroethane	Cl_3CCCl_3	236.74	1, 87	2.091		187	sublimes	none	s alc, bz, chl, eth
h28	1,4,5,6,7,7-Hexachloro-5-norbornene-2,3-di-carboxylic anhydride		370.83	9^3, 4049			239–242			
h29	Hexachlorophene	$CH_3[C_6H(Cl)_3OH]_2$	406.91	6^3, 5407			163–165		none	
h30	Hexachloropropene	$Cl_3CC(Cl)=CCl_2$	248.75	1, 200	1.765	1.5480^{20}		210	none	
h31	Hexadecane	$CH_3(CH_2)_{14}CH_3$	226.45	1, 172	0.7733_4^{20}	1.4345^{20}	18.2	286.8	135	misc eth
h32	1,2-Hexadecanediol	$CH_3(CH_2)_{13}CH(OH)CH_2OH$	258.45	1^3, 2244			72–74			
h33	1-Hexadecanethiol	$CH_3(CH_2)_{15}SH$	258.51	1, 430	0.840	1.4720^{20}	18–20	184^{7mm}	101	sl s alc, s eth
h34	Hexadecanoic acid	$CH_3(CH_2)_{14}CO_2H$	256.43	2, 370	0.852_4^{62}	1.4273^{80}	62	351		s hot: chl, eth
h35	1-Hexadecanol	$CH_3(CH_2)_{15}OH$	242.45	1, 429	0.8116^{60}	1.4355^{60}	49.3	334	135	s alc, chl, eth
h36	1-Hexadecene	$CH_3(CH_2)_{14}CH=CH_2$	224.43	1, 226	0.783_4^{20}	1.4401	4.1	284	132	s alc, eth, PE
h37	1-Hexadecylamine	$CH_3(CH_2)_{15}NH_2$	241.46	4, 202			45–48	330	140	v s alc, eth; s bz, chl
h38	2,4-Hexadienal	$CH_3CH=CHCH=CHCHO$	96.13	1^2, 809	0.871	1.5386^{20}		76^{30mm}	67	
h39	1,5-Hexadiene	$H_2C=CHCH_2CH_2CH=CH_2$	82.15	1, 253	0.6923_4^{20}	1.4042^{20}	−140.7	59.5	−27	s alc, eth
h40	2,4-Hexadienoic acid	$CH_3CH=CHCH=CO_2H$	112.13	2, 483			134.5	119^{10mm}	127	0.2 aq; 13 alc; 9 acet; 2.3 bz; 11 diox; 1 CCl_4
h41	Hexafluorobenzene	C_6F_6	186.05	5^3, 523	1.6182^{20}	1.3781^{20}	5.1	80.3	10	
h42	Hexafluoroethane	F_3CCF_3	138.01	1^3, 132	1.590^{-78}		−100.7	−78.3		sl s alc, eth
h43	1,1,1,3,3,3-Hexafluoro-2-propanol	$(CF_3)_2CHOH$	168.04		1.596^{25}	1.2750^{20}	−3	58.2	none	s aq, bz, CCl_4
h44	Hexafluoropropene	$CF_3CF=CF_2$	150.02	1^3, 697			−153	−28		
h45	Hexamethylcyclotri-siloxane	$[-Si(CH_3)_2O-]_3$	222.48	4^3, 1884			64–66	133–135	35	
h46	1,1,1,3,3,3-Hexamethyl-disilazane	$(CH_3)_3SiNHSi(CH_3)_3$	161.40	4,*3*, 1861	0.774_4^{20}	1.4071^{20}		126	8	
h47	Hexamethyldisiloxane	$(CH_3)_3SiOSi(CH_3)_3$	162.38	4^3, 1859	0.764_4^{20}	1.3775^{20}	−67	101	−2	
h48	Hexamethyleneimine		99.18	20, 94	0.880	1.4631^{20}		138^{749mm}	18	

h49	Hexamethylene-tetramine		140.19	1, 583	1.331^{-5}		280 subl		250	67 aq; 8 alc; 10 chl
h50	Hexamethyl-phosphoramide	$[(CH_3)_2N]_3P(=O)$	179.20		1.027^{20}	1.4588^{20}	7	232^{740mm}	105	misc aq
h51	Hexanaldehyde	$CH_3(CH_2)_4CHO$	100.16	1^2, 745	0.8335_4^{20}	1.4035^{20}	−56	131	32	v s alc, eth; sl s aq
h52	Hexane	$CH_3(CH_2)_4CH_3$	86.18	1, 142	0.6594_4^{20}	1.3749^{20}	−95.4	68.7	−22	misc alc, chl, eth
h53	1,6-Hexanediamine	$H_2N(CH_2)_6NH_2$	116.21	4, 269			42	205	81	v s aq; sl s alc, bz
h54	1,6-Hexanedioic acid	$HO_2C(CH_2)_4CO_2H$	146.14	2, 649	1.360_4^{25}		152–154	337.5	196	1.4 aq; v s alc; s acet
h55	**DL**-1,2-Hexanediol	$CH_3(CH_2)_3CH(OH)CH_2OH$	118.18	1^1, 251	0.951	1.4425^{20}		223–224	>110	
h56	1,6-Hexanediol	$HO(CH_2)_6OH$	118.18	1, 484	0.958	1.4579^{25}	42.8	208	101	v s aq, alc
h57	2,5-Hexanediol	$CH_3CH(OH)CH_2CH_2CH(OH)CH_3$	118.18	1, 485	0.9617_{16}^{45}	1.4465^{20}	−50	220.8	101	s aq, alc, eth
h58	1,6-Hexanediol diacrylate	$[H_2C{=}CHCO_2(CH_2)_{3-}]_2$	226.28		1.010	1.4562^{20}			>110	
h59	1,6-Hexanediol dimethacrylate	$[H_2C{=}C(CH_3)CO_2(CH_2)_{3-}]_2$	254.33		0.995	1.4580^{20}		> 350	>110	
h60	2,5-Hexanedione	$CH_3C(=O)CH_2CH_2C(=O)CH_3$	114.14	1, 788	0.973_4^{20}	1.4260^{20}	−9	188	78	misc aq, alc, eth
h61	Hexanenitrile	$CH_3(CH_2)_4CN$	97.16	2, 324	0.8052^{20}	1.4069^{20}	−80.3	163.6	43	i aq; s alc, eth
h62	1-Hexanethiol	$CH_3(CH_2)_5SH$	118.24	1^3, 1659	0.8424_4^{20}	1.4496^{20}	−80.5	152.7	20	i aq; v s alc, eth
h63	1,2,6-Hexanetriol	$HOCH_2CH(OH)(CH_2)_3CH_2OH$	134.17	1^4, 2784	1.1063_{20}^{20}	1.58^{20}	−32.8	178^{5mm}	191	misc alc, acet; i bz

Hexachloro-2-propanone, h21
$\alpha,\alpha,\alpha,\alpha',\alpha',\alpha'$-Hexachloro-*p*-xylene, b225
Hexadecyl mercaptan, h33
$\alpha,\alpha,\alpha,\alpha',\alpha',\alpha'$-Hexafluoro-3,5-xylidine, h229
Hexahydroaniline, c375
Hexahydro-2*H*-azepin-2-one, o61
Hexahydrobenzaldehyde, c352
Hexahydrobenzene, c347
Hexahydrobenzoic acid, c353
Hexahydrobenzylamine, c362
Hexahydrophthalic acid, c356
Hexahydropyridine, p180
Hexamethylenediamine, h53
Hexamethylene diisocyanate, d461
Hexamethylene glycol, h56
Hexamethylethane, t100
2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosene, s8
1,6,10,15,19,23-Hexamethyltetracosane, s7
1,6-Hexanedinitrile, d284
6-Hexanelactam, o61



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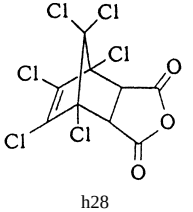

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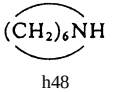

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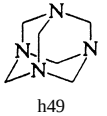

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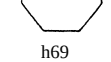
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
h64	Hexanoic acid	$CH_3(CH_2)_4CO_2H$	116.16	2, 321	0.9265_4^{20}	1.4168^{20}	−3	205	102	1.1 aq; v s alc, eth
h65	Hexanoic anhydride	$[CH_3(CH_2)_4C(=O)]_2O$	214.31	2, 324	0.926	1.4280^{20}	−41	246–248	>110	s alc
h66	1-Hexanol	$CH_3(CH_2)_5OH$	102.18	1, 407	0.8136^{20}	1.4182^{20}	−44.6	157.5	63	8 aq; misc bz, eth; s alc
h67	2-Hexanol	$CH_3(CH_2)_3CH(OH)CH_3$	102.18	1, 408	0.8108_4^{25}	1.4128^{25}	−47	139.9	41	sl s aq; s alc, eth
h68	3-Hexanol	$CH_3CH_2CH_2CH(OH)CH_2CH_3$	102.18	1, 408	0.8193_4^{20}	1.4160^{20}		135	41	
h69	6-Hexanolactone		114.14	17^2, 290	1.030	1.4630^{20}	−18	215	109	
h70	2-Hexanone	$CH_3(CH_2)_3C(=O)CH_3$	100.16	1, 689	0.8113^{20}	1.4007^{20}	−55.5	127.6	25	v s alc, eth
h71	3-Hexanone	$CH_3CH_2CH_2C(=O)CH_2CH_3$	100.16	1, 690	0.815	1.4002^{20}		123	35	
h72	Hexanoyl chloride	$CH_3(CH_2)_4C(=O)Cl$	134.61	2, 324	0.9754_4^{20}	1.4263^{20}	−87	153	50	dec aq, alc; s eth
h73	1-Hexene	$CH_3(CH_2)_3CH=CH_2$	84.16	1, 215	0.6732^{20}	1.3879^{20}	−139.8	63.5	−9	0.005 aq
h74	*trans*-2-Hexenoic acid	$CH_3(CH_2)_2CH=CHCO_2H$	114.14	2^4, 1563	0.965	1.4885^{20}	33–35	217	>110	
h75	*trans*-3-Hexenoic acid	$CH_3CH_2CH=CHCH_2CO_2H$	114.14	2, 435	0.963	1.4398^{20}	11–12	119^{22mm}	>110	
h76	*trans*-2-Hexen-1-ol	$CH_3CH_2CH_2CH=CHCH_2OH$	100.16	1^2, 486	0.849	1.4343^{20}		158–160	54	
h77	5-Hexen-2-one	$H_2C=CHCH_2CH_2C(=O)CH_3$	98.15	1, 734	0.847	1.4197^{20}		128–129	23	
h78	*trans*-2-Hexenyl acetate	$CH_3C(=O)CH_2CH=CHCH_2$-CH_2CH_3	142.20	2^2, 151	0.898	1.4275^{20}		166	58	
h79	Hexyl acetate	$CH_3(CH_2)_5O_2CCH_3$	144.21	2, 132	0.860_{20}^{20}	1.4090^{20}	−81	171	45	0.13 aq; v s alc, eth
h80	Hexyl acrylate	$H_2C=CHCO_2(CH_2)_5CH_3$	156.23	2^3, 1228	0.888	1.4280^{20}		90^{24mm}	68	
h81	Hexylamine	$CH_3(CH_2)_5NH_2$	101.19	4, 188	0.763_4^{25}	1.4180^{20}	−23	133	8	sl s aq; misc alc, eth
h82	1-Hexyne	$CH_3(CH_2)_3C\equiv CH$	82.14	1, 253	0.7152_4^{20}	1.3989^{20}	−131.9	71.3	−21	i aq; s alc, eth
h83	L-Histidine		155.16	25, 513			282 dec			41 aq; v sl s alc
h84	Hydantoin		100.08	24, 242			221–223			s alc, alk; sl s eth
h85	Hydrazine	H_2NNH_2	32.05	Merck: 12, 4809	1.0036_4^{25}	1.4700^{20}	1.4	113.5	52	misc aq, alc
h86	1,4-Hydroquinone	C_6H_4-1,4-$(OH)_2$	110.11	6, 836	1.332^{15}		172	286		7 aq; v s alc, eth; sl s bz
h87	Hydroxyacetaldehyde	$HOCH_2CHO$	60.05	1, 817	1.366^{100}		93–94	110^{12mm}		v s aq, alc; sl s eth
h88	Hydroxyacetic acid	$HOCH_2CO_2H$	76.05	3, 228			80	100		s aq, alc, acet, eth
h89	1′-Hydroxy-2′-aceto-naphthone	$C_{10}H_6(OH)C(=O)CH_3$	186.21	8, 149			98–100	325 sl d		i aq; v s bz; s HOAc
h90	Hydroxyacetone	$HOCH_2C(=O)CH_3$	74.08	1^1, 84	1.082	1.4315^{20}	−17	146	56	misc aq, alc, eth

h91	2′-Hydroxyaceto-phenone	$HOC_6H_4C(=O)CH_3$	136.15	8, 85	1.131_4^{21}	1.5584^{20}	4–6	213^{717mm}	>110	misc alc, eth; sl s aq
h92	3′-Hydroxyaceto-phenone	$HOC_6H_4C(=O)CH_3$	136.15	8, 86	1.100^{100}	1.535^{100}	87–89	296		s aq; v s alc, bz, eth
h93	4′-Hydroxyaceto-phenone	$HOC_6H_4C(=O)CH_3$	136.15	8, 87	1.109^{100}		109–111	148^{3mm}		v s alc, eth; sl s aq
h94	2-Hydroxybenz-aldehyde	$C_6H_4(OH)CHO$	122.12	8, 31	1.1674^{20}	1.5740^{20}	−7	196.7	78	1.7 aq[86]; s alc, eth
h95	3-Hydroxybenz-aldehyde	$C_6H_4(OH)CHO$	122.12	8, 58			103–105	191^{50mm}		s alc, bz, eth; sl s aq
h96	4-Hydroxybenz-aldehyde	$C_6H_4(OH)CHO$	122.12	8, 64	1.129_4^{130}		117–119			1 aq; 70 acet; 4 bz[65]; v s alc, eth
h97	2-Hydroxybenz-aldehyde oxime	$C_6H_4(OH)CH{=}NOH$	137.14	8, 49			57	dec		v s alc, bz, eth, acids
h98	2-Hydroxybenzamide	$C_6H_4(OH)C(=O)NH_2$	137.14	10, 87			140	dec 270		0.2 aq; s alc, chl, eth
h99	2-Hydroxybenzoic acid	$C_6H_4(OH)CO_2H$	138.12	10, 43	1.443_4^{20}		157–159	211^{20mm}		0.2 aq; 37 alc; 33 eth; 33 acet; 2 chl; 0.7 bz

D-*erythro*-Hex-2-enonic acid γ-lactone, i69
Hexyl alcohol, h66
sec-Hexyl alcohol, e95
sec-Hexylamine, m371
Hexylbenzene, p116
Hexyl bromide, b346
Hexyl chloride, c149
Hexylene glycol, m360
Hexyl iodide, i36
Hexyl methyl ketone, o36
Hexyl propyl ketone, d20
Hippuric acid, b70
Homocysteine, a200
Homopiperidine, h48
Homoveratric acid, d513
Homoveratrylamine, d517
Hydroacrylonitrile, h173
2-Hydrazinoethanol, h125
Hydrazobenzene, d757
Hydrindene, i10
Hydrocinnamic acid, p150
Hydroquinone, d430
Hydroquinone dimethyl ether, d495
Hydroxyacetanilides, a15 thru a17
Hydroxybenzene, p65
2-Hydroxybenzenemethanol, h107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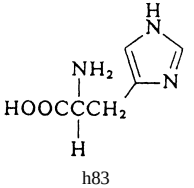
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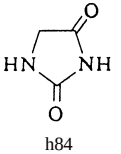
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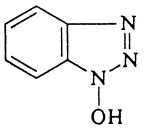
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
h100	3-Hydroxybenzoic acid	$C_6H_4(OH)CO_2H$	138.12	10, 134	1.473		201–203			0.8 aq; 10 eth
h101	4-Hydroxybenzoic acid	$C_6H_4(OH)CO_2H$	138.12	10, 149	1.468^{4}		215–217			0.2 aq; v s alc; 23 eth
h102	4-Hydroxybenzoic hydrazide	$HOC_6H_4C(=O)NHNH_2$	152.15	10, 174			266 dec			
h103	4-Hydroxybenzophenone	$HOC_6H_4C(=O)C_6H_5$	198.22	8^{2}, 184			132–135			v s alc, eth; sl s aq
h104	1-Hydroxybenzotriazole		135.13	26, 41			155–158			
h105	6-Hydroxy-1,3-benzoxathiol-2-one		168.17	19^{4}, 2508			158–160			
h106	2-Hydroxybenzyl alcohol	$HOC_6H_4CH_2OH$	124.13	6, 891	1.161^{25}		83–85	subl 100		6.6 aq; v s alc, chl, eth; s bz
h107	1-Hydroxy-2-butanone	$CH_3CH_2C(=O)CH_2OH$	88.11	1, 826	1.026	1.4282^{20}		78^{60mm}	60	
h108	3-Hydroxy-2-butanone	$CH_3C(=O)CH(OH)CH_3$	88.11	1, 827	0.9972_{4}^{17}	1.4171^{20}	15	148	50	misc aq, alc; sl s eth
h109	4-Hydroxycinnamic acid	$HOC_6H_4CH{=}CHCO_2H$	164.16	10, 297			210–213			s alc, eth; sl s aq
h111	7-Hydroxycoumarin		162.14	18, 27			226–228			v s alc, chl, alk, HOAc
h112	1-Hydroxy-1-cyclohexanecarbonitrile	$C_6H_{10}(OH)CN$	125.17	10, 5	1.031	1.4576^{20}	29		60	
h113	2-Hydroxy-3,5-diiodobenzoic acid	$I_2C_6H_2(OH)CO_2H$	389.91	10, 113			232–235			v s alc, eth; i bz, chl
h114	4-Hydroxy-3,5-dinitrobenzoic acid	$HOC_6H_2(NO_2)CO_2H$	228.12	1, 183			245 dec			
h115	3-Hydroxydiphenylamine	$HOC_6H_4NHC_6H_5$	185.23	13, 410			80–82	340		
h116	(2-Hydroxydiphenyl)methane	$HOC_6H_4CH_2C_6H_5$	184.24	6, 675		1.5994^{20}	54	312	>110	s organic solvents, alk
h117	(4-Hydroxydiphenyl)methane	$HOC_6H_4CH_2C_6H_5$	184.24	6, 675			84	322		s hot aq, org solvents, HOAc, alkalis

h118	2-(2-Hydroxyethoxy)-phenol	$HOCH_2CH_2C_6H_4OH$	154.17	6^2, 782			99–100	$128^{0.7mm}$		
h119	*N*-(2-Hydroxyethyl)-acetamide	$HOCH_2CH_2NHC(=O)CH_3$	103.12	4^1, 430	1.1233_{20}^{20}	1.4575^{20}	63–65	155^{5mm}	176	misc aq; sl s bz
h120	2-Hydroxyethyl acetate	$CH_3CO_2CH_2CH_2OH$	104.11	2, 141	1.108^{15}	1.4201^{20}		188	88	misc aq, alc, chl, eth
h121	2-Hydroxyethyl acrylate	$H_2C{=}CHCO_2CH_2CH_2OH$	116.12	2^4, 1469	1.011	1.4500^{20}		92^{12mm}	98	
h122	3-(1-Hydroxyethyl)-aniline	$CH_3CH(OH)C_6H_4NH_2$	137.18	13^3, 1654			66–69			
h123	2-Hydroxyethyl disulfide	$HOCH_2CH_2SSCH_2CH_2OH$	154.25	1, 471	1.261	1.5655^{20}	25–27	$158^{3.5mm}$	>110	
h124	*N*-(2-Hydroxyethyl)-ethylenediamine-*N*,*N*,*N*′-triacetic acid	$HO_2CCH_2N(CH_2CH_2OH)$-$CH_2CH_2N(CH_2CO_2H)_2$	278.26				212 dec			
h125	2-Hydroxyethyl-hydrazine	$HOCH_2CH_2NHNH_2$	76.10	4^1, 562	1.123	1.4961^{20}	−70	220	73	misc aq; s alc
h126	2-Hydroxyethyl methacrylate	$HOCH_2CH_2O_2CC(CH_3){=}CH_2$	130.14		1.073	1.4520^{20}		$67^{3.5mm}$	97	
h127	*N*-(2-Hydroxyethyl)-morpholine		131.18	27, 7	1.083	1.4760^{20}		227	99	misc aq
h128	*N*-(2-Hydroxyethyl)-phthalimide		191.19	21, 469			126–128			
h129	1-(2-Hydroxyethyl)-piperazine		130.19	23^2, 6	1.061	1.5065^{20}		246	>110	

m-Hydroxybenzotrifluoride, t304
Hydroxybutanedioic acids, h186, h187
5-Hydroxydecanoic acid, δ-lactone, d17
Hydroxyethanal, h87
3-(α-Hydroxyethyl)aniline, a256
N-(2-Hydroxyethyl)-3-aza-1,5-pentanediol, t266
N-(2-Hydroxyethyl)ethyleneimine, a311
N-(2-Hydroxyethyl)piperidine, p182
2-(2-Hydroxyethyl)piperidine, p183



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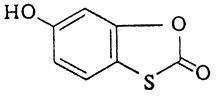

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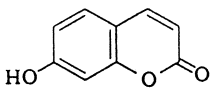

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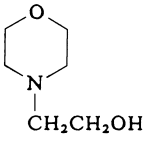

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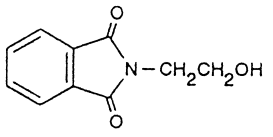

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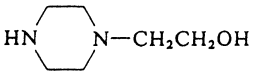

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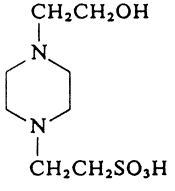
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
h130	*N*-(2-Hydroxyethyl)-piperazine-*N′*-ethane-sulfonic acid		238.31	Merck: 12, 4687			234 dec			sat'd aq: 2.25*M*[0]
h131	*N*-(2-Hydroxyethyl)-piperidine		129.20	20, 25	1.0059_4^{15}	1.4804^{20}		199–202	68	
h132	*N*-(2-Hydroxyethyl)-pyridine	$HOCH_2CH_2NC_5H_4$	123.16	21, 50	1.093	1.5368^{20}		116^{9mm}	92	v s aq, alc, chl
h133	*N*-(2-Hydroxyethyl)-pyrrolidine	$HOCH_2CH_2NC_4H_8$	115.8	20^2, 5	0.985	1.4713^{20}		81^{13mm}	56	
h134	*N*-(2-Hydroxyethyl)-2-pyrrolidinone		129.16	21^4, 3142	1.143	1.4960^{20}		142^{2mm}	>110	
h135	2-Hydroxyethyl salicylate	$(HO)C_6H_4CO_2CH_2CH_2OH$	182.18	10, 81	1.224	1.5480^{20}		166^{13mm}	>110	
h136	(2-Hydroxyethyl)triphenylphosphonium bromide	$HOCH_2CH_2P(C_6H_5)_3Br$	387.26	16, 761			217–219			
h137	8-Hydroxy-7-iodo-5-quinolinesulfonic acid		351.12	22, 408			269–270 dec			
h138	2-Hydroxyisobutyric acid	$(CH_3)_2C(OH)CO_2H$	104.11	3, 313			82	$84^{1.5mm}$		v s aq, alc, eth
h138a	2-Hydroxyisobutyronitrile	$(CH_3)_2C(OH)CN$	85.11	3, 316	0.932	1.3990^{20}	−19	82^{23mm}	63	
h139	Hydroxylamine HCl	$H_2NOH \cdot HCl$	69.49		1.670		159 dec			
h140	4-Hydroxy-2-mercapto-6-methylpyrimidine		142.18	24, 351			330 dec			v s aq NH_3, alkalis; sl s alc, acet
h141	4-Hydroxy-2-mercapto-6-propylpyrimidine		170.23				219–221			0.1 aq; 1.7 alc; 1.7 acet; v s alkalis
h142	4-Hydroxy-3-methoxybenzaldehyde	$CH_3OC_6H_3(OH)CHO$	152.15	8, 247	1.056		80–81	285		1 aq; s alc, chl, pyr
h143	4-Hydroxy-3-methoxybenzoic acid	$CH_3OC_6H_3(OH)CO_2H$	168.15	10, 392			210–213			0.12 aq; v s alc

h144	2-Hydroxy-4-methoxy-benzophenone	$CH_3OC_6H_3(OH)C(=O)C_6H_5$	228.25	8, 312			63–66	160^{5mm}		v s alc, chl, eth
h145	4-Hydroxy-3-methoxy-benzyl alcohol	$CH_3OC_6H_3(OH)CH_2OH$	154.17	6, 1113			113–115			
h146	*N*-(Hydroxymethyl)-acrylamide	$H_2C{=}CHC(=O)NHCH_2OH$	101.11	2^4, 1472	1.074	1.430^{20}			none	
h147	4-Hydroxy-3-methyl-2-butanone	$HOCH_2CH(CH_3)C(=O)CH_3$	102.13	1^1, 422	0.993	1.4340^{20}		92^{15mm}	81	
h148	7-Hydroxy-4-methyl-coumarin		176.17	18, 31			190–192			s alc, HOAc; sl s eth
h149	*N*-(Hydroxymethyl)-nicotinamide	$(C_5H_4N)C(=O)NHCH_2OH$	152.15	10, 4750			152–154			
h150	4-Hydroxy-4-methyl-2-pentanone	$(CH_3)_2C(OH)CH_2C(=O)CH_3$	116.16	Merck: 12, 3008	0.9306^{25}_4	1.4235^{20}	−44	167.91	58	misc aq
h151	*N*-(Hydroxymethyl)-phthalimide		177.16	21, 475			147–149			sl s aq, alc, bz

Hydroxyhydroquinone, b34
2-Hydroxyisobutyronitrile, h153
2-Hydroxy-3-methyl-2-cyclopenten-1-one, m223
(2-Hydroxymethyl)-2-nitro-1,3-propanediol, t442
1,3-Hydroxy-2-methyl-2-propylamine, a226



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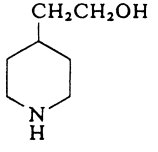

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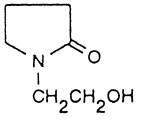

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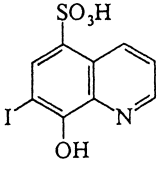

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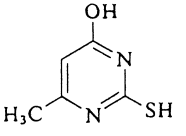

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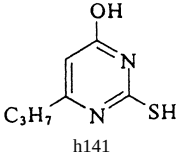

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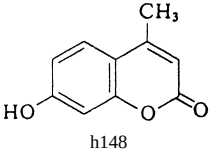

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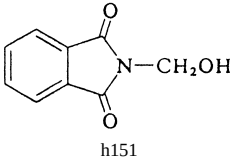


h151

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

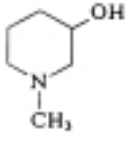
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
h152	4-Hydroxy-*N*-methyl-piperidine		115.18	21^{1}, 188		1.4775^{20}	29–31	200		
h153	2-Hydroxy-2-methyl-propionitrile	$(CH_3)_2C(OH)CN$	85.10	3, 316	0.9267^{25}_{4}	1.3992^{20}	−19	95	63	s aq, alc, chl, eth
h154	2-Hydroxy-2-methyl-propiophenone	$C_6H_5C(=O)C(CH_3)_2OH$	164.20	8^{1}, 553	1.077	1.5330^{20}		103^{4mm}	>110	
h155	5-Hydroxy-2-methyl-pyridine	$HO(C_5H_2N)CH_3$	109.13	21^{3}, 480			168–170			
h156	3-Hydroxy-2-methyl-4-pyrone		126.11				161–162			1.2 aq; v s hot aq; s alc, alk; sl s bz, eth
h157	2-Hydroxy-1-naphth-aldehyde	$C_{10}H_6(OH)CHO$	172.18	8, 143			82–85	192^{27mm}		
h158	1-Hydroxy-2-naphthoic acid	$C_{10}H_6(OH)CO_2H$	188.18	10, 331			191–192			v s alc, bz, eth, alk
h159	2-Hydroxy-1-naphthoic acid	$C_{10}H_6(OH)CO_2H$	188.18	10, 328			167 dec			
h160	3-Hydroxy-2-naphthoic acid	$C_{10}H_6(OH)CO_2H$	188.18	10, 333			222–223			v s alc, eth; s bz, chl
h161	2-Hydroxy-1,4-naphthoquinone		174.16	8, 300			dec >191			s HOAc
h162	4-Hydroxy-3-nitro-benzenearsonic acid	$HOC_6H_3(NO_2)AsO(OH)_2$	263.04	16^{1}, 456			>300			v s alc, acet, HOAc, alk; sl s aq; i eth
h163	4-Hydroxy-3-nitro-benzoic acid	$HOC_6H_3(NO_2)CO_2H$	183.12	10, 181			184–185			
h164	5-Hydroxy-2-pentanone	$CH_3C(=O)CH_2CH_2CH_2OH$	102.13	1, 831	1.007^{20}_{4}	1.4372^{20}		144^{100mm}	93	misc aq; s alc, eth
h165	4-Hydroxyphenylacetic acid	$HOC_6H_4CH_2CO_2H$	152.15	10, 190			149–151			v s alc, eth; sl s aq
h166	4-(4-Hydroxyphenyl)-2-butanone	$HOC_6H_4CH_2CH_2C(=O)CH_3$	164.20	8^{2}, 117			82–83			
h167	4-Hydroxyphenyl-glycine	$HOC_6H_4CH(NH_2)CO_2H$	167.16	14^{1}, 659			240 dec			sl s aq, alc, bz, acet

h168	*N*-(4-Hydroxyphenyl)-glycine	$HOC_6H_4NHCH_2CO_2H$	167.16	13, 488			244 dec			s alk, acid; v sl s aq, alc, acet, bz, eth
h169	2′-Hydroxy-3-phenyl-propiophenone	$HOC_6H_4C(=O)CH_2CH_2C_6H_5$	226.28	8^{2}, 202		1.5968^{20}	36–37		>110	
h170	1-(3-Hydroxyphenyl)-urea	$HOC_6H_4NHC(=O)NH_2$	152.15	13, 417			182–184			
h171	*N*-Hydroxyphthalimide		163.13	21, 500			233 dec			
h172	2-Hydroxypropionitrile	$CH_3CH(OH)CN$	71.08	3^{2}, 209	0.9834^{25}	1.4027^{25}	−40	103^{50mm}	76	misc aq, alc; s eth
h173	3-Hydroxypropionitrile	$HOCH_2CH_2CN$	71.08	3, 298	1.0404^{25}_{4}	1.4248^{20}	−46	221	129	misc aq, alc, acet; 2,3 eth; i bz, PE
h174	2′-Hydroxypropio-phenone	$HOC_6H_4C(=O)CH_2CH_3$	150.18	8, 102	1.094	1.5480^{20}		115^{15mm}	>110	v s alc, eth; sl s aq
h175	4′-Hydroxypropio-phenone	$HOC_6H_4C(=O)CH_2CH_3$	150.18	8, 102			148			v s alc, eth; sl s aq
h176	1-(2-Hydroxy-1-propoxy)-2-propanol	$CH_3CH(OH)CH_2OCH_2$-$CH(OH)CH_3$	134.18		1.0252^{20}_{20}	1.4440^{20}		231.8	138	misc aq, alc
h177	Hydroxypropyl acrylate	$H_2C{=}CHCO_2(CH_2)_3OH$	130.14	2^{4}, 1469	1.044	1.4450^{20}		77^{5mm}	89	
h178	Hydroxypropyl methacrylate	$H_2C{=}C(CH_3)CO_2(CH_2)_3OH$	144.17	2^{4}, 1532	1.066	1.4470^{20}		$57^{0.5mm}$	96	
h179	2-Hydroxypyridine	HOC_5H_4N	95.10	21, 43			105–107	280–281		aq, alc, bz, sl s eth
h180	3-Hydroxypyridine	HOC_5H_4N	95.10			126–129		151^{3mm}		v s aq, alc; sl s eth
h181	4-Hydroxypyridine	HOC_5H_4N	95.18					230^{12mm}		v s aq; i alc, bz, eth

1-Hydroxy-2-naphthalenecarboxylic acid, h158
2-Hydroxy-1-naphthalenecarboxylic acid, h159
3-Hydroxy-2-naphthalenecarboxylic acid, h160
6-Hydroxynicotinic acid, h182
Hydroxynitroanilines, a238, a239, a240

α-Hydroxy-*α*-phenylacetophenone, b46
3-(*p*-Hydroxyphenyl)alanine, t455
2-Hydroxy-2-phenylbenzeneacetic acid, b37
3-Hydroxy-1-propanesulfonic acid γ-sultone, p197
2-Hydroxypropanoic acid, L1, L2

1-Hydroxy-2-propanone, h90
3-Hydroxypropionitrile, c323
1-(2-Hydroxy-1-propoxy)-2-propanol, b204
3-Hydroxy-1-propyne, p249



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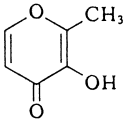

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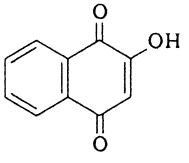

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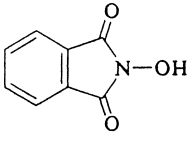


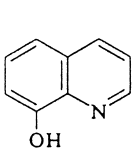
h171

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
h182	2-Hydroxypyridine-5-carboxylic acid	$HO(C_5H_3N)CO_2H$	139.11	22, 215			>300			sl s aq, alc, eth
h183	3-Hydroxypyridine-*N*-oxide	$(HO)C_5H_4N{=}O$	111.10				190–192			
h184	8-Hydroxyquinoline		145.16	21, 91			72–74	267^{742mm}		v s alc, acet, bz, chl
h185	8-Hydroxyquinoline-5-sulfonic acid		225.22	22, 407			>300			v s aq; sl s alc, eth
h186	**DL**-Hydroxysuccinic acid	$HO_2CCH(OH)CH_2CO_2H$	134.09	3, 435			131–133			56 aq; 45 EtOH; 18 acet; 0.8 eth; 23 diox
h187	(−)-Hydroxysuccinic acid	$HO_2CCH(OH)CH_2CO_2H$	134.09	3, 419			100			36 aq; 87 EtOH; 61 acet; 2.7 eth; 75 diox
h188	*N*-Hydroxysuccinimide		115.09	21, 380			95–98			v s aq
i1	Icosane	$CH_3(CH_2)_{18}CH_3$	282.56	1, 174	0.7777^{37}	1.4346^{40}	36.4	343.8	>112	
i2	1-Icosene	$CH_3(CH_2)_{17}CH{=}CH_2$	280.54	1^3, 881			28.7	342.4		
i3	1*H*-Imidazole		68.08	23, 45			90–91	257	145	v s aq, alc, chl, eth
i4	2-Imidazolidinethione		102.16	24,4			203–204			2 aq; s alc, pyr; i bz, acet, chl, eth
i5	2-Imidazolidone		86.09	24, 16			133–135			v s aq, hot alc
i6	3,3′-Iminobis(*N*,*N*-dimethyl)propylamine	$HN[(CH_2)_3N(CH_3)_2]_2$	187.33	4^3, 565	0.841	1.4490^{20}	−78	131^{20mm}	98	
i7	Iminodiacetic acid	$HO_2CCH_2NHCH_2CO_2H$	133.10	4, 365			243 dec			2 aq; v sl s bz, eth
i8	Iminodiacetonitrile	$NCCH_2NHCH_2CN$	95.11	4, 367			77			s aq, alc; sl s eth
i9	Iminodibenzyl		195.27				105–108			
i10	Indane		118.18	Merck: 12, 4966	0.9639_4^{20}	1.5383^{20}	−51.4	178	50	s alc, chl, eth; i aq
i11	5-Indanol		134.18	6, 575			51–53	255	>110	v s alc, eth; sl s aq
i12	1-Indanone		132.16	7, 360	1.1090_4^{45}	1.561^{45}	40–42	243–245	111	s alc, eth; sl s aq
i13	1,2,3-Indantrione hydrate		178.14	Merck: 12, 6645			dec 241			v s aq; s alc
i14	Indene		116.16	5, 515	0.9968_4^{20}	1.5762^{20}	−1.8	181.6	58	misc alc, bz, chl, eth
i15	Indole		117.15	20, 304	1.0643	1.609^{60}	52.54	253–254	>110	s hot aq, bz, eth
i16	Indole-3-acetic acid		175.19	22, 66			168–170			v s alc; s acet, eth

i17	Indole-2,3-dione		147.13	21, 432			203.5 dec			s hot aq, hot alc, alk
i18	Indoline		119.17	20, 257	1.063	1.5906^{20}		221	92	sl s aq
i19	Inositol		180.16	6^{2}, 1157	1.752		225			14 aq; sl s alc; i eth
i20	Iodoacetamide	ICH_2CONH_2	184.96	2, 223			93–96			s hot aq
i21	Iodoacetic acid	ICH_2CO_2H	185.95	2, 222			79–82			s aq, alc; v sl s eth

Icosane, e1
Imidodicarbonic diamide, b238
Imidole, p279
Indalone, b450
Indanamine, a195, a196
Indonaphthene, i14
5-Iodoanthranilic acid, a199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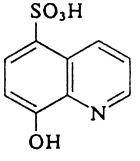
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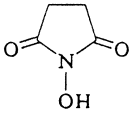
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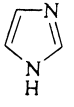
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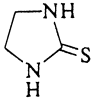
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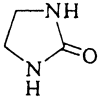
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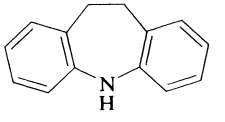
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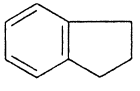
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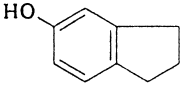
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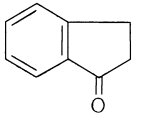
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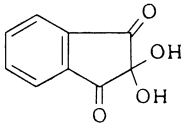
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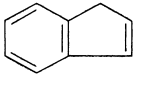
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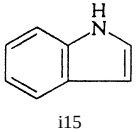
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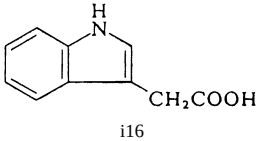
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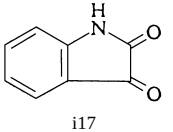
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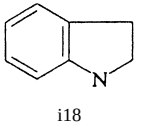
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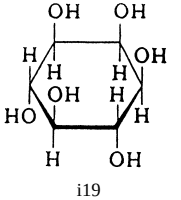
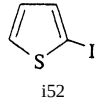

i19

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
i22	3-Iodoaniline	$IC_6H_4NH_2$	219.03	12, 670	1.821	1.6820^{20}	25	146^{15mm}	>110	i aq; s alc, eth
i23	Iodobenzene	C_6H_5I	204.01	5, 215	1.8308^{20}	1.6200^{20}	−31	188	74	misc alc, chl, eth
i24	Iodobenzene diacetate	$C_6H_5I(O_2CCH_3)_2$	322.10	5, 218			163–165			
i25	2-Iodobenzoic acid	$IC_6H_4CO_2H$	248.02	9, 363	2.249_4^{25}		162–164			s alc, eth; sl s aq
i26	1-Iodobutane	$HC_3CH_2CH_2CH_2I$	184.02	1, 123	1.6154^{20}	1.4999^{20}	−103.5	130–131	33	i aq; s alc, eth
i27	2-Iodobutane	$CH_3CH_2CH(I)CH_3$	184.02	1, 123	1.5920^{20}	1.4991^{20}	−104.0	120	23	i aq; s alc, eth
i28	Iodocyclohexane	$C_6H_{11}I$	210.06	5[2], 13	1.626_{15}^{15}	1.5472^{20}		180		i aq; s eth
i29	1-Iododecane	$CH_3(CH_2)_9I$	268.19	1, 168	1.257_4^{20}	1.4850^{20}		132^{15mm}	>110	i aq; s alc, eth
i30	2-Iodododecane	$CH_3(CH_2)_{11}I$	296.24	1[1], 67	1.201	1.4844	−3	160^{15mm}	>110	
i31	Iodoethane	CH_3CH_2I	155.97	1, 96	1.9358^{20}	1.5130^{20}	−111	72.4	none	0.4 aq; misc alc, bz, chl, eth
i32	2-Iodoethanol	ICH_2CH_2OH	171.97	1, 339	2.2197_4^{20}	1.5694^{20}		75^{5mm}	65	s aq; v s alc, eth
i33	Iodoform	CHI_3	393.73	1, 73	4.008		120–123		none	1.4 alc; 10 chl; 13 eth; v s bz, acet
i34	1-Iodoheptane	$CH_3(CH_2)_6I$	226.10	1, 155	1.373_4^{20}	1.4900^{20}	−48	204	78	i aq; s alc, eth
i35	1-Iodohexadecane	$CH_3(CH_2)_{15}I$	352.35	1, 172	1.121	1.4806^{20}	23	207^{10mm}	>110	
i36	1-Iodohexane	$CH_3(CH_2)_5I$	212.08	1, 146	1.437_4^{20}	1.4920^{20}		179–180	61	i aq
i37	1-Iodomethane	CH_3I	141.94	1, 69	2.2789_4^{20}	1.5308^{20}	−66.5	42.5	none	1.4 aq; misc alc, eth
i38	1-Iodo-2-methyl-propane	$(CH_3)_2CHCH_2I$	184.02	1, 128	1.6035^{20}	1.4960^{20}	−93.5	121	12	i aq; misc alc, eth
i39	2-Iodo-2-methyl-propane	$(CH_3)_3CI$	184.02	1[3], 326	1.571_0^0	1.4918^{20}	−38	100	7	dec aq; misc alc, eth
i40	1-Iodo-3-nitrobenzene	$IC_6H_4NO_2$	249.01	5, 253	1.9477_4^{50}		36–38	280	71	i aq; s alc, eth
i41	1-Iodo-4-nitrobenzene	$IC_6H_4NO_2$	249.01	5, 252			175–177	289^{772mm}	>110	
i42	1-Iodononane	$CH_3(CH_2)_8I$	254.18	1, 166	1.288	1.4870^{20}		108^{8mm}	85	
i43	1-Iodooctadecane	$CH_3(CH_2)_{17}I$	380.40	1, 173			33–35	197^{2mm}	>110	
i44	1-Iodooctane	$CH_3(CH_2)_7I$	240.13	1, 160	1.330_4^{20}	1.4889^{20}	−46	226	95	s alc, eth
i47	1-Iodopentane	$CH_3(CH_2)_4I$	198.06	1, 133	1.512_4^{20}	1.4954^{20}	−85	155	51	sl s aq; s alc, eth
i48	1-Iodopropane	$CH_3CH_2CH_2I$	169.99	1, 113	1.7489^{20}	1.5058^{20}	−101	102	44	0.1 aq; misc alc, eth
i49	2-Iodopropane	$(CH_3)_2CHI$	169.99	1, 114	1.7042^{20}	1.4992^{20}	−90	89.5	42	0.14 aq; misc alc, eth
i50	3-Iodo-1-propene	$ICH_2CH{=}CH_2$	167.97	1, 202	1.845_4^{22}	1.5540^{21}	−99	103	18	misc alc, chl, eth
i51	5-Iodosalicylic acid	$IC_6H_3(OH)CO_2H$	264.02	10, 112			189–191			v s alc; i bz, chl

i52	2-Iodothiophene		210.04	17, 34	1.902	1.6520^{20}	−40	73^{15mm}	71	v s eth
i53	2-Iodotoluene	$IC_6H_4CH_3$	218.04	5, 310	1.713	1.6079^{20}		211	90	i aq; s alc, eth
i54	3-Iodotoluene	$IC_6H_4CH_3$	218.04	5, 311	1.698	1.6040^{20}		82^{10mm}	82	i aq; misc alc, eth
i55	4-Iodotoluene	$IC_6H_4CH_3$	218.04	5, 312			34–36	211	90	
i56	Iodotrimethylsilane	$(CH_3)_3SiI$	200.10		1.406_4^{20}	1.4710^{20}		106	−31	
i57	1-Iodoundecane	$CH_3(CH_2)_{10}I$	282.21	1[1], 66	1.220	1.4849^{20}		130^{5mm}	>110	
i58	*α*-Ionone		192.30	7, 168	0.932^{20}	1.4980^{20}		124^{11mm}	104	s alc, bz, chl, eth
i59	*β*-Ionone		192.30	7, 167	0.946^{17}	1.521^{17}		128^{12mm}	>110	s alc, bz, chl, eth
i60	Isatoic anhydride		163.13	27, 264			233 dec			sl s aq, hot alc, acet
i61	**D**-(−)-Isoascorbic acid		176.12				169 dec			s aq, alc, acet, pyr
i62	**DL**-Isoborneol		154.25	6[2], 80			214 subl			v s alc, chl, eth
i63	Isobutyl acetate	$(CH_3)_2CHCH_2O_2CCH_3$	116.16	2, 131	0.8712^{20}	1.3902^{20}	−99	116.5	18	0.7 aq; v s alc
i64	Isobutyl acetoacetate	$CH_3COCH_2CO_2CH_2CH(CH_3)_2$	158.20		0.980	1.4240^{20}		100^{22mm}	78	
i65	Isobutyl acrylate	$H_2C{=}CHCO_2CH_2CH(CH_3)_2$	128.19	2[3], 1227	0.890	1.4140		132	32	
i66	Isobutylamine	$(CH_3)_2CHCH_2NH_2$	73.14	4, 163	0.724_4^{20}	1.3972^{20}	−86.6	68	−9	misc aq, alc, acet, eth
i67	Isobutylbenzene	$C_6H_5CH_2CH(CH_3)_2$	134.22	5, 414	0.8532^{20}	1.4866^{20}	−51.5	172.8	55	misc alc, eth
i68	Isobutyl chloroformate	$ClCO_2CH_2CH(CH_3)_2$	136.58	3, 12	1.053	1.4070^{20}		128.8	27	misc bz, chl, eth
i69	Isobutyl formate	$HCO_2CH_2CH(CH_3)_2$	102.13	2, 21	0.8776^{20}	1.3855^{20}	−95.5	98.4	10	1 aq; misc alc, eth
i70	Isobutyl isobutyrate	$(CH_3)_2CHCH_2O_2CH(CH_3)_2$	144.22	2, 291	0.8542^{20}	1.3999^{20}	−80.7	148.5	38	0.5 aq; misc alc
i71	Isobutyl methacrylate	$H_2C{=}C(CH_3)CO_2CH_2CH(CH_3)_2$	142.19	2[3], 1287	0.882_{15}^{25}	1.4170^{25}		155	41	misc alc, eth

Isatin, i17
Isoamyl acetate, i91
Isoamyl alcohol, m163
sec-Isoamyl alcohol, m164
Isoamyl bromide, b362
Isoamyl chloride, c169a
Isoamyl nitrite, i92
1,3-Isobenzofurandione, p169
Isobutane, m390
Isobutene, m399
α-Isobutoxy-*α*-phenylacetophenone, b48
Isobutylacetylene, m372
Isobutyl alcohol, m397
Isobutyl bromide, b371
Isobutyl chloride, c179
Isobutyl chlorocarbonate, i68
Isobutyl ether, d458
Isobutyl mercaptan, m395
Isobutyl methyl ketone, m370



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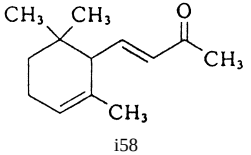

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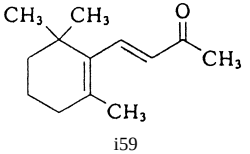

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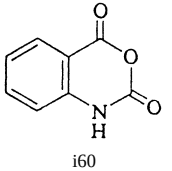

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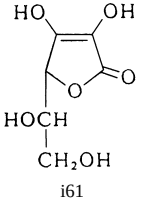

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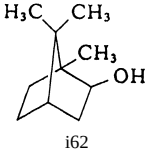


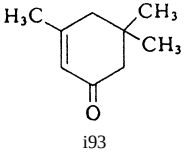
i62

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
i72	Isobutyl nitrate	$(CH_3)_2CHCH_2ONO_2$	119.12	1, 377	1.015_4^{20}	1.4028^{20}		123	21	i aq; misc alc, eth
i73	Isobutyl nitrite	$(CH_3)_2CHCH_2ONO$	103.12	1, 377	0.870_4^{22}	1.3715^{22}		67	−21	misc alc; sl s aq (dec)
i74	Isobutyl propionate	$C_2H_5CO_2CH_2CH(CH_3)_2$	130.19	2, 241	0.888_4^0	1.3974^{20}	−71	137	26	i aq; misc alc
i75	Isobutyl stearate	$CH_3(CH_2)_{16}CO_2CH_2CH(CH_3)_2$	340.57				*ca.* 20			
i76	Isobutyltriethoxysilane	$(CH_3)_2CHCH_2Si(OC_2H_5)_3$	220.39		0.880	1.400^{20}		190–191	60	
i77	Isobutyltrimethoxysilane	$(CH_3)_2CHCH_2Si(OCH_3)_3$	178.30		0.930	1.3960^{20}		137	39	
i78	Isobutyl vinyl ether	$(CH_3)_2CHCH_2OCH{=}CH_2$	100.16	1^3, 1862	0.7702_{20}^{20}	1.3950^{20}	−112	83.4	−13	0.2 aq
i79	Isobutyraldehyde	$(CH_3)_2CHCHO$	72.11	1, 671	0.7988_4^{20}	1.3723^{20}	−65.9	64.5	−18 (CC)	11 aq; misc alc, bz, acet, chl, eth
i80	Isobutyramide	$(CH_3)_2CHCONH_2$	87.12	2, 293	1.013		127–129	216–220		
i81	Isobutyric acid	$(CH_3)_2CHCO_2H$	88.11	2, 288	0.9681^{20}	1.3925^{20}	−46	154	56	17 aq; misc alc, chl, eth
i82	Isobutyric anhydride	$[(CH_3)_2CHCO]_2O$	158.20	2, 292	0.954	1.4062^{20}	−56	182	59	
i83	Isobutyronitrile	$(CH_3)_2CHCN$	69.11	2, 294	0.7704^{20}	1.3720^{20}	−71.5	104	8	v s alc, eth; sl s aq
i84	Isobutyrophenone	$C_6H_5COCH(CH_3)_2$	148.21	7, 316	0.988^{20}	1.5172		217	84	
i85	Isobutyryl chloride	$(CH_3)_2CHCOCl$	106.55	2, 293	1.017	1.4073^{20}	−90	91–93	1	dec aq, dec alc; s eth
i86	Isodecyl acrylate	$H_2C{=}CHCO_2C_{10}H_{21}$	212.34		0.875	1.4420^{20}		121^{10mm}	106	
i87	Isodecyl methacrylate	$H_2C{=}C(CH_3)CO_2C_{10}H_{21}$	226.36		0.878	1.4430^{20}		126^{10mm}	>110	
i88	L-Isoleucine	$C_2H_5CH(CH_3)CH(NH_2)CO_2H$	131.18	4, 454			288 dec	subl 168		4 aq; sl s hot alc
i89	Isooctyl acrylate	$H_2C{=}CHCO_2C_8H_{17}$	184.25		0.880	1.4370^{20}		125^{20mm}	80	
i90	Isooctyl diphenyl phosphite	$(C_6H_5O)_2POC_8H_{17}$	346.41		1.045	1.5220^{20}		188		
i91	Isopentyl acetate	$CH_3CO_2CH_2CH_2CH(CH_3)_2$	130.19	2, 132	0.876_4^{15}	1.4007^{20}	−78.5	142	25	0.25 aq; misc alc, eth
i92	Isopentyl nitrite	$ONOCH_2CH_2CH(CH_3)_2$	117.15	1, 402	0.872	1.3860^{20}		99	10	misc alc, eth; sl s aq
i93	Isophorone		138.21	7, 65	0.955^{20}	1.4759^{20}	−8.1	215.2	84	1.2 aq
i94	Isophorone diisocyanate		222.29		1.049	1.4841^{20}		159^{15mm}	>110	
i95	Isopropenyl acetate	$CH_3CO_2C(CH_3){=}CH_2$	100.12	2^2, 278	0.909	1.4005^{20}		94	18	
i96	3-Isopropenyl-α,α-dimethylbenzyl isocyanate	$H_2C{=}C(CH_3)C_6H_4C(CH_3)_2NCO$	201.27		1.108	1.5300^{20}		268–271	>110	
i97	2-Isopropoxyethanol	$(CH_3)_2CHOCH_2CH_2OH$	104.15	1^2, 519	0.903	1.4104^{20}		44^{13mm}	45	

i98	3-Isopropoxypropyl-amine	$(CH_3)_2CHO(CH_2)_3NH_2$	117.19	4^3, 739	0.845	1.4195^{20}		79^{85mm}	39	
i99	Isopropyl acetate	$(CH_3)_2CHO_2CCH_3$	102.13	2, 130	0.8718^{20}	1.3770^{20}	−73	89	2	3 aq; misc alc, eth
i100	Isopropylamine	$(CH_3)_2CHNH_2$	59.11	4, 152	0.686_4^{25}	1.3711^{25}	−95	31.7	−37	misc aq, alc, eth
i101	2-Isopropylaniline	$(CH_3)_2CHC_6H_4NH_2$	135.2	12, 1147	0.955	1.5477^{20}		222	95	
i102	4-Isopropyl-benzaldehyde	$(CH_3)_2CHC_6H_4CHO$	148.21	7, 318	0.977	1.5298^{20}		236	93	
i103	Isopropylbenzene	$(CH_3)_2CHC_6H_5$	120.20	5, 393	0.864_4^{20}	1.4915^{20}	−96	152–154	36	s alc, bz, eth
i104	4-Isopropylbenzyl alcohol	$(CH_3)_2CHC_6H_4CH_2OH$	150.22	6, 543	0.982^{15}	1.5206^{20}	28	248.4	>110	misc alc, eth; i aq
i105	*N*-Isopropylbenzyl-amine	$C_6H_5CH_2NHCH(CH_3)_2$	149.24		0.892	1.5025^{20}		200	87	
i106	Isopropyl butyrate	$CH_3CH_2CH_2CO_2CH(CH_3)_2$	130.19	2, 271	0.859	1.3932^{20}		131	30	
i107	Isopropyl chloro-acetate	$ClCH_2CO_2CH(CH_3)_2$	136.58	2, 198	1.096	1.4190^{20}		149–150	70	
i108	Isopropylcyclohexane	$C_6H_{11}CH(CH_3)_2$	126.24	5, 41	0.8023_4^{20}	1.4399^{20}	−90	155	35	v s alc, eth

Isobutyl octadecanoate, i75
Isobutyraldehyde, m389
Isobutyric acid, m402
Isocapronitrile, m361
Isocinchomeronic acid, p269
Isocrotonic acid, b483
Isocumene, p225
5-Isocyanato-1-(isocyanatomethyl)-1,3,3-trimethylcyclohexane, i94
Isodurene, t98
Isoeugenol, m108
Isohexane, m357
Isoleucinol, a211
Isomesityl oxide, m370
Isonicotinaldehyde, p263
Isonicotinic acid, p267
Isonicotinonitrile, c330
Isooctane, t381
Isopentane, m158
Isopentyl alcohol, m163
Isopentyl isopentanoate, m177
Isopentyl isovalerate, m177
Isophorone, t364
Isophthalic acid, b17
Isophthalonitrile, d283
Isophthaloyl dichloride, b15
Isoprene, m157
Isopropanolamine, a263
Isopropenyl acetate, p207
Isopropenylacetylene, m174
Isopropenyl methyl ether, m106
Isopropylacetylene, m178
Isopropylacrylic acid, m369
Isopropyl alcohol, p202
Isopropyl bromide, b401
Isopropyl chloride, c226
Isopropyl cyanide, i83
Isopropylethanol, m164
Isopropyl ether, d476
Isopropylethylene, m167



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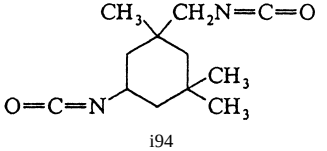


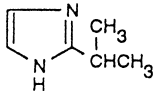
i94

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
i109	Isopropyl hexadecanoate	$CH_3(CH_2)_{14}CO_2CH(CH_3)_2$	298.51	2^2, 336	0.862	1.4385^{20}			>110	
i110	4,4′-Isopropylidene-bis(2,6-dibromo-phenoxy)ethanol	$(CH_3)_2C[C_6H_2(Br)_2OCH_2CH_2OH]_2$	632.01				107			
i111	4,4′-Isopropylidene-bis(diisodecyl phenyl phosphite)	$[(C_{10}H_{21}O)_2POC_6H_4]_2C(CH_3)_2$	917.34		0.964	1.4980^{20}		336	>110	
i112	4,4′-Isopropylidene-dicyclohexanol	$(CH_3)_2C(C_6H_{10}OH)_2$	240.39	6^2, 761				234^{14mm}	>110	
i113	4,4′-Isopropylidene-diphenol	$(CH_3)_2C(C_6H_4OH)_2$	228.29	6, 1011			137–140	220^{4mm}		
i114	2-Isopropylimidazole		110.16	23, 83			129–131	256–260		
i115	Isopropyl isocyanate	$(CH_3)_2CHCNO$	85.11	4, 155	0.866	1.3825^{20}		74–75	−2	
i116	Isopropyl *S*-(−)-lactate	$(CH_3)_2CHO_2CCH(OH)CH_3$	132.16	3, 282	0.998^{20}_{20}	1.4082^{25}		166–168	57	s aq, alc, eth
i117	2-Isopropyl-6-methyl-aniline	$(CH_3)_2CHC_6H_3(CH_3)NH_2$	149.24		0.957	1.5440^{20}			41	
i118	2-Isopropyl-1-methyl-benzene	$(CH_3)_2CHC_6H_4CH_3$	134.21	5, 419	0.8766^{20}_4	1.5006^{20}	−71.5	178.2		misc alc, eth
i119	3-Isopropyl-1-methyl-benzene	$(CH_3)_2CHC_6H_4CH_3$	134.21	5, 419	0.8610^{20}_4	1.4930^{20}	−63.8	175.1		misc alc, eth
i120	4-Isopropyl-1-methyl-benzene	$(CH_3)_2CHC_6H_4CH_3$	134.21	5, 420	0.8573^{20}_4	1.4909^{20}	−68.9	177.1	47	misc alc, eth
i121	2-Isopropyl-5-methyl-phenol	$(CH_3)_2CHC_6H_3(CH_3)OH$	150.22	6, 532	0.925^{80}_4		51.5	232.5		i aq; v s alc, chl, eth
i122	4-Isopropyl-3-methyl-phenol	$(CH_3)_2CHC_6H_3(CH_3)OH$	150.22	6^2, 491			111–114			
i123	5-Isopropyl-3-methyl-phenol	$(CH_3)_2CHC_6H_3(CH_3)OH$	150.22	6, 526			51		>110	
i124	Isopropyl nitrate	$(CH_3)_2CHONO_2$	105.09	1, 363	1.036^{19}_{19}	1.391^{20}		102	12	
i125	Isopropyl nitrite	$(CH_3)_2CHONO$	89.09	Merck: 12, 5235	0.844^{25}_4	1.3520^{20}		39^{752mm}		
i126	1-Isopropyl-4-nitro-benzene	$(CH_3)_2CHC_6H_4NO_2$	165.19	5^2, 308	1.090	1.5380^{20}		107^{11mm}	>110	

i127	2-Isopropylphenol	$(CH_3)_2CHC_6H_4OH$	136.19	6, 504	1.012^{20}	1.5259^{20}	15–16	212–213	88	misc alc, eth
i128	3-Isopropylphenol	$(CH_3)_2CHC_6H_4OH$	136.19	6, 505	0.994	1.5250^{20}	25	228	104	
i129	4-Isopropylphenol	$(CH_3)_2CHC_6H_4OH$	136.19	6, 505	0.990^{20}		59–61	212		316 alc; 350 eth
i130	4-Isopropylpyridine	$(CH_3)_2CH(C_5H_4N)$	121.18	20, 248	0.938	1.4980^{20}		173	66	
i131	Isopropyl tetradecanoate	$(CH_3)_2CHO_2C(CH_2)_{12}CH_3$	270.46	2^3, 923	0.850	1.4350^{20}	*ca.* 3	193^{20mm}	>110	s caster oil, cottonseed oil, acet, EtOAc, EtOH, toluene, mineral oil
i132	Isopulegol		154.25	6, 65	0.912	1.4725^{20}		91^{12mm}	78	v sl s aq
i133	Isoquinoline		129.16	20, 380	1.0910_4^{30}	1.6208^{30}	26.5	243.5	107	sl s aq; s acid
k1	Ketene	$H_2C{=}C{=}O$	42.04	1, 724			−151	−49.8		s acet, eth; dec aq
k2	8-Ketotricyclo-[5.2.1.$0^{2,6}$]decane		150.22	7^2, 133	1.063	1.5020^{20}		132^{30mm}	101	
L1	**DL**-Lactic acid	$CH_3CH(OH)CO_2H$	90.08	3, 268	1.249_4^{15}		16.8	122^{14mm}	>110	s aq, alc; i chl, PE
L2	**L**-(+)-Lactic acid	$CH_3CH(OH)CO_2H$	90.08	3, 261	1.2060_4^{25}	1.4270^{20}	53	119^{12mm}	>110	v s aq, alc, eth
L3	α-Lactose		342.32	31, 408			202			20 aq; v sl s alc

Isopropylidone acetone, m370
Isopropyl iodide, i49
Isopropyl mercaptan, p199
1-Isopropyl-4-methyl-1,3-cyclohexadiene, t10
2-Isopropyl-5-methylcyclohexanol, m12
1-Isopropyl-4-methyl-1,4-cyclohexadiene, t11
Isopropyl methyl ketone, m165
Isopropyl myristate, i131
Isopropyl palmitate, i109
Isopropyltoluenes, i118, i119, i120
Isopseudocumenol, t385
Isovaleraldehyde, m181
Isovaleric acid, m184
Isovaleronitrile, m185
Isovaleryl chloride, m186
Itaconic acid, m253
Keto-, *see* oxo-
2-Ketobutyric acid, o60
5-Keto-1,7,7-trimethylnorcamphane, c3
4-Ketovaleric acid, o63
Lactonitrile, h172



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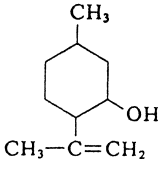

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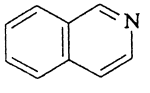

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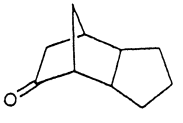
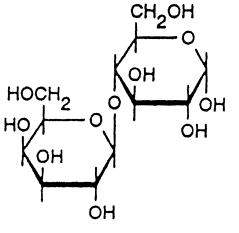


k2



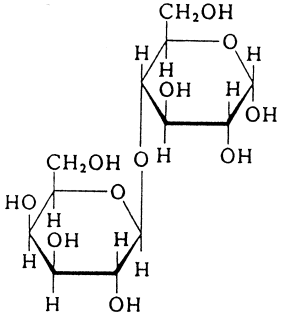
L3

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
L4	*β*-Lactose		342.32	31, 408	1.525^{20}		202			45 aq; i alc, eth
L5	**DL**-Leucine	$(CH_3)_2CHCH_2CH(NH_2)CO_2H$	131.18	4, 447			dec 332	subl 293		1 aq; 0.13 alc; i eth
L6	**L**-Leucine	$(CH_3)_2CHCH_2CH(NH_2)CO_2H$	131.18	4, 437	1.293^{18}		293 dec	subl 145		2.4 aq[25]; 0.07 alc; 1 HOAc; i eth
L7	*R*-(+)-Limonene		136.24	5, 133	0.8411_4^{20}	1.4730	−96.5	178	49	misc alc, eth
L8	*S*-(−)-Limonene		136.24	5, 136	0.841_4^{20}	1.4746^{20}	−96.5	178	48	misc alc, eth
L9	(+)-Limonene oxide		152.24	17, 44	0.929	1.4661^{20}		114^{50mm}	65	
L10	Linalool		154.25	1, 462	0.865^{15}	1.4615^{20}		197^{720mm}	76	misc alc, eth
L11	Linalyl acetate		196.29	2, 141	0.895_4^{20}	1.4460^{20}		220	90	misc alc, eth
L12	*S*-(+)-Lysine	$H_2N(CH_2)_4CH(NH_2)CO_2H$	146.19	4, 435			212 dec			v s aq; sl s alc; i eth
m1	Maleic acid	$HO_2CH{=}CHCO_2H$	116.07	2, 748	1.590		130.5			70 aq; 70 alc; s acet, HOAc; sl s eth
m2	Maleic anhydride		98.06	17, 432	1.48		52.8	202	103	s aq (to acid), alc (to ester); 227 acet; 53 chl; 50 bz; 112 EtOAc
m3	Malonic acid	$HO_2CCH_2CO_2H$	104.06	2, 566	1.63		135–137			154 aq; 42 alc; 8 eth; 14 pyr
m4	Malonodiamide	$H_2NCOCH_2CONH_2$	102.09	2, 582			172–175			9 aq; i alc, eth
m5	Malononitrile	$NCCH_2CN$	66.06	2, 589	1.1910_4^{20}	1.4146^{34}	32–34	220	112	13 aq, 40 alc; 20 eth
m6	Malonyl dichloride	$ClCOCH_2COCl$	140.95	2[1], 252	1.4486_4^{19}	1.4620^{20}		55^{19mm}	47	dec hot aq; s eth
m7	**D**-(+)-Maltose hydrate		360.32	31, 386	1.540^{17}		119–121	dec 130		v s aq; sl s alc; i eth
m8	**DL**-Mandelic acid	$C_6H_5CH(OH)CO_2H$	152.15	10, 192	1.300_4^{20}		120–122			16 aq; 100 alc; s eth
m9	Mandelonitrile	$C_6H_5CH(OH)CN$	133.15	10, 193	1.117	1.5315^{20}	−10	170	97	v s alc, cho, eth; i aq
m10	Mannitol		182.17	1, 534	1.52^{20}		166–168	$290^{3.5mm}$		18 aq; 1.2 alc; i eth
m11	**D**-(+)-Mannose		180.16	31, 284	1.54^{20}		128–130			250 aq; 28 pyr; 0.8 alc
m12	(−)-Menthol		156.27	6, 28	0.890_{15}^{15}	1.458^{25}	41–43	212	93	v s alc, chl, eth, PE
m13	(−)-Menthone		154.25	7, 38	0.895_4^{20}	1.4510^{20}	−6	207	72	misc alc, eth; sl s aq
m14	*S*-(+)-Menthyl acetate		198.31	6, 32	1.4480^{20}			229–230	77	

Lauraldehyde, d817
Lauric acid, d809
Lauryl alcohol, d810
Laurylamine, d818
Lauryl bromide, b327
Lauryl mercaptan, d808
Lauryl methacrylate, d819
Lauryl sulfate, d820
Lepidine, m421
Leucinol, a212
Levulinic acid, o63
Limonene, m313a
Linoleic acid, o1
Linolenic acid, o7
Luminol, a151
2,6-Lupetidine, d672
β-Lutidine, e257
Lutidines, d685 thru d689
Maleic hydrazide, d447
Malic acid, h186, h187
Malonaldehyde bis(dimethyl acetal), t92
Malonamide nitrile, c319
Malonic acid diamide, m4
Malonylurea, b1
Margaryl alcohol, h1a
Mellitic acid, b20
MEM chloride, m74
Menadione, m321
1,8-Mentanediamine, d51
p-Mentha-1,8-diene, L17, L18
p-Mentha-6,8-dien-2-one, c20
Mercaptobenzene, t156

1.253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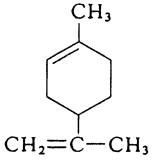
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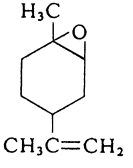
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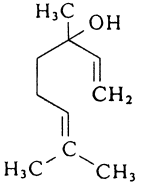
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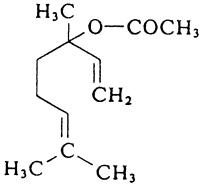
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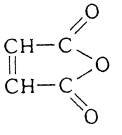
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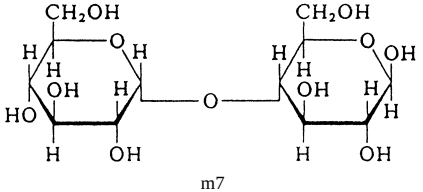
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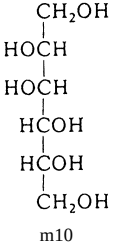
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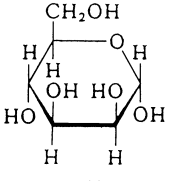
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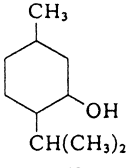
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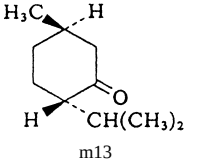
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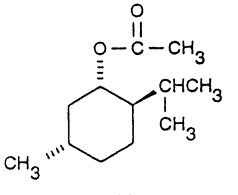
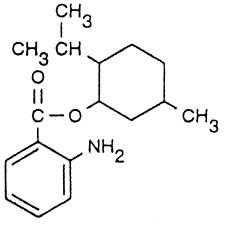

m14

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

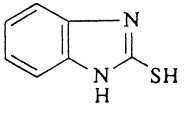
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
m15	Menthyl anthranilate		275.40	14^{3}, 885	1.040	1.5420^{20}		179^{3mm}	>110	
m16	Mercaptoacetic acid	$HSCH_2CO_2H$	92.12	3, 245	1.325	1.5030^{20}	−16.5	96^{5mm}	>110	misc aq, alc, bz, eth
m17	2-Mercaptobenz-imidazole		150.20	24, 119			301–305			sl s aq; s alc
m18	2-Mercaptobenzoic acid	$HSC_6H_4CO_2H$	154.19	10, 125			165–168			v s alc, HOAc
m19	2-Mercaptobenzo-thiazole		167.25	27, 185	1.42_4^{20}		180–181	dec		2 alc; 1 eth; 10 acet; 1 bz; s alk; i aq
m20	2-Mercaptoethanol	$HSCH_2CH_2OH$	78.13	1, 470	1.1143_4^{20}	1.5006^{20}		156.9	73	misc aq, alc, bz, eth
m21	3-Mercapto-1,2-propanediol	$HSCH_2CH(OH)CH_2OH$	108.16	1, 519	1.295_{14}^{14}	1.5243^{20}		118^{5mm}	>110	misc alc; v s acet
m22	2-Mercaptopropionic acid	$CH_3CH(SH)CO_2H$	106.14	3, 289	1.220_4^{15}	1.4809^{20}	10–14	102^{16mm}	87	misc aq, alc, eth, acet
m23	3-Mercaptopropionic acid	$HSCH_2CH_2CO_2H$	106.14	3, 299	1.218	1.4911^{20}	17–19	111^{15mm}	93	
m24	(3-Mercaptopropyl)-trimethoxysilane	$HS(CH_2)_3Si(OCH_3)_3$	196.34		1.039_4^{20}	1.4440^{20}		198	48	
m25	Mercaptosuccinic acid	$HO_2CCH_2CH(SH)CO_2H$	150.15	3, 439			5–7			50 aq; 50 alc; s eth
m26	2-Mercaptothiazoline		119.21	27, 140			105–107			
m27	Methacrylaldehyde	$H_2C{=}C(CH_3)CHO$	70.09	1, 731	0.847	1.4160^{20}	−81	69	−15	6 aq; misc alc, eth
m28	Methacrylamide	$H_2C{=}C(CH_3)CONH_2$	85.11	2^{2}, 399			109–111			s alc; sl s eth
m29	Methacrylic acid	$H_2C{=}C(CH_3)CO_2H$	86.09	2, 421	1.0153_4^{20}	1.4314^{20}	16	163	77	9 aq; misc alc, eth
m30	Methacrylic anhydride	$[H_2C{=}C(CH_3)CO]_2O$	154.17	2^{3}, 1293	1.035	1.4530^{20}		87^{13mm}	84	
m30a	Methacrylonitrile	$H_2C{=}C(CH_3)CN$	67.91	2, 423	0.8001_4^{20}	1.4007^{20}	−35.8	90.3	1.1	2.6 aq; misc acet, bz
m31	Methacryloyl chloride	$H_2C{=}C(CH_3)COCl$	104.54	2^{2}, 394	1.070	1.4420^{20}		95–96	2	
m32	Methallylidene diacetate	$(CH_3CO_2)_2CHC(CH_3){=}CH_2$	172.18	2^{4}, 292	1.039	1.4245^{20}	−15	191	83	
m33	Methane	CH_4	16.04	1, 56	0.7168 g/L 0.4240^{bp}		−182.5	−161.5		3.3 mL aq; 47 mL alc
m34	Methanesulfonic acid	CH_3SO_3H	96.10	4, 4	1.4812_4^{18}	1.4303^{20}	20	167^{10mm}	>110	1.5 bz; misc aq
m35	Methanesulfonic anhydride	$(CH_3SO_2)_2O$	174.19	4, 5			71	138^{10mm}		v s aq (dec)
m36	Methanesulfonyl chloride	CH_3SO_2Cl	114.55	4, 5	1.4805_4^{18}	1.4518^{20}	−32	161	>110	s alc, eth

m37	Methanethiol	CH_3SH	48.11	1, 288	1.966 g/L		−123	6.0		2.3 aq; v s alc, eth
m38	Methanol	CH_3OH	32.04	1, 273	0.7913_4^{20}	1.3284^{20}	−97.7	64.7	11	misc aq, alc, bz, chl, eth
m39	Methanol-*d*	CH_3OD	33.05	1^3, 1186	0.8127_4^{20}	1.3270^{20}	−110	65.5	11	misc aq, alc, eth
m40	Methanol-d_4	CD_3OD_1	36.07	1^3, 1187	0.888	1.3256^{20}		65.4	11	misc aq, alc, eth
m41	Methanol-^{13}C	$^{13}CH_3OH$	33.03	1^3, 1187	0.815	1.3290^{20}	−97.8	64	12	
m42	**DL**-Methionine	$CH_3SCH_2CH_2CH(NH_2)CO_2H$	149.21	4^2, 938	1.340		281 dec			3 aq; i eth; v sl s alc
m43	Methoxyacetic acid	$CH_3OCH_2CO_2H$	90.08	3, 232	1.174	1.4158^{20}		202–204	>110	misc aq, alc, eth
m44	2′-Methoxyacetophenone	$CH_3OC_6H_4COCH_3$	150.18	8, 85	1.090_4^{20}	1.5393^{20}		131^{18mm}	108	
m45	3′-Methoxyacetophenone	$CH_3OC_6H_4COCH_3$	150.18	8, 86	1.094	1.5410^{20}		239–241	>110	s aq
m46	4′-Methoxyacetophenone	$CH_3OC_6H_4COCH_3$	150.18	8, 87	1.082_4^{41}	1.5335	36–38	154^{26mm}	>110	v s alc, eth
m47	3-Methoxyacrylonitrile	$CH_3OCH{=}CHCN$	83.09		0.990	1.4550^{20}			76	
m48	2-Methoxyaniline	$CH_3OC_6H_4NH_2$	123.16	13, 358	1.098_{15}^{15}	1.5730^{20}	5–6	225	98	i aq; misc alc, eth
m49	3-Methoxyaniline	$CH_3OC_6H_4NH_2$	123.16	13, 404	1.096	1.5794^{20}	−10	251	>110	s alc, acid; sl s aq
m50	4-Methoxyaniline	$CH_3OC_6H_4NH_2$	123.16	13, 435	1.087		57–60	240–243		v s alc; sl s aq

Mesidine, t335
Mesitol, t387
Mesitylene, t359
Mesityl oxide, m370
Mesoxylurea, a73
Mesyl chloride, m36
Metanilic acid, a116
Methacholine chloride, a49
Methacrolein, m27
Methacrolein diacetate, m32
Methallyl alcohol, m400
Methallyl chloride, c182
Methanal, f31
Methanoic acid, f36
Methenamine, h49
Malononitrile dimer, a267
Methone, d596
Methoxyacetaldehyde dimethyl acetal, t340



m15



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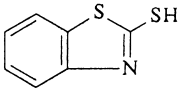

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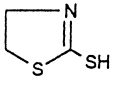


m26

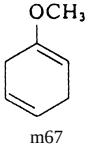
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
m51	2-Methoxybenz-aldehyde	$CH_3OC_6H_4CHO$	136.15	8, 43	1.127	1.560^{20}	37–39	238	117	sl s alc, bz; i eth
m52	3-Methoxybenz-aldehyde	$CH_3OC_6H_4CHO$	136.15	8, 59	1.119	1.5533^{20}		143^{50mm}	>110	
m53	4-Methoxybenz-aldehyde	$CH_3OC_6H_4CHO$	136.15	8, 67	1.119	1.5713^{20}	−1	248	108	misc alc
m54	4-Methoxybenzamide	$CH_3OC_6H_4CONH_2$	151.17	10^2, 100			164–167	295	108	s aq; v s alc; sl s eth
m55	Methoxybenzene	$CH_3OC_6H_5$	108.14	6, 138	0.9942^{20}	1.5170^{20}	−37.5	153.8	51	1 aq; misc alc, eth
m56	4-Methoxybenzene-sulfonyl chloride	$CH_3OC_6H_4SO_2Cl$	206.65	11, 243			40–43		>110	dec aq; s alc, eth
m57	2-Methoxybenzoic acid	$CH_3OC_6H_4CO_2H$	152.15	10, 64	1.180		100	200		0.5 aq; v s alc, eth
m58	3-Methoxybenzoic acid	$CH_3OC_6H_4CO_2H$	152.15	10, 137			104	172^{10mm}		s hot aq, alc, eth
m59	4-Methoxybenzoic acid	$CH_3OC_6H_4CO_2H$	152.15	10, 154	1.385^4		185	275–280		0.04 aq; v s alc, chl
m60	4-Methoxybenzoyl chloride	$CH_3OC_6H_4COCl$	170.60	10, 163		1.5810^{20}	22	145^{14mm}	87	i aq (dec); s alc (dec); s acet, bz
m61	4-Methoxybenzyl alcohol	$CH_3OC_6H_4CH_2OH$	138.17	6, 897	1.109_4^{25}	1.5442^{20}	23–25	259	>110	i aq; s alc, eth
m62	4-Methoxybenzylamine	$CH_3OC_6H_4CH_2NH_2$	137.18	13, 606	1.050^{15}	1.5462^{20}		236–237	>110	v s aq, alc, eth
m63	2-Methoxybiphenyl	$CH_3OC_6H_4C_6H_5$	184.24	6, 672	1.023	1.6105^{20}	30–33	274	>110	
m64	3-Methoxy-1-butanol	$CH_3OCH(CH_3)CH_2CH_2OH$	104.15		0.9229_{20}^{20}	1.4145^{20}	−85	161.1	46	misc aq
m65	4-Methoxy-3-buten-2-one	$CH_3OCH{=}CHCOCH_3$	100.12		0.982	1.4680^{20}		200	63	
m66	2-Methoxycinnam-aldehyde	$CH_3OC_6H_4CH{=}CHCHO$	162.19				44–48	$130^{0.6mm}$	>110	
m67	1-Methoxy-1,4-cyclo-hexadiene		110.16	6^3, 367	0.940	1.4819^{20}		148–150	36	
m68	2-Methoxydibenzo-furan		198.22	17^3, 1590			42–45		>110	
m69	7-Methoxy-3,7-dimethyloctanal	$(CH_3)_2C(OCH_3)(CH_2)_3$-$CH(CH_3)CH_2CHO$	186.30		0.877	1.4374^{20}		$60^{0.45mm}$	98	
m70	2-Methoxy-1,3-dioxolane		104.11	19^4, 617	1.092	1.4091^{20}		129–130	31	

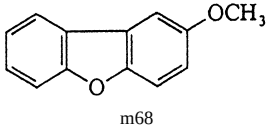
m71	2-Methoxyethanol	$CH_3OCH_2CH_2OH$	76.10	1, 467	0.9646^{20}	1.4021^{20}	−85.1	124	39	misc aq
m72	2-(2-Methoxyethoxy)-acetic acid	$CH_3OCH_2CH_2OCH_2CO_2H$	134.13	3^3, 374	1.180	1.4380^{20}		245–250	>110	
m73	2-(2-Methoxyethoxy)-ethanol	$CH_3OCH_2CH_2OCH_2CH_2OH$	120.15		1.035_4^{20}	1.4264^{20}	−50	194	96	misc aq, alc, bz, eth, ketones
m74	2-Methoxyethoxy-methyl chloride	$CH_3OCH_2CH_2OCH_2Cl$	124.57		1.091	1.4270^{20}		50^{13mm}	>110	
m75	2-Methoxyethyl acetate	$CH_3CO_2CH_2CH_2OCH_3$	118.13	2, 141	1.0049^{20}	1.4002^{20}	−70	144	49	misc aq
m76	2-Methoxyethyl acetoacetate	$CH_3COCH_2CO_2CH_2CH_2OCH_3$	160.17		1.090	1.4339^{20}		120^{20mm}	103	
m77	2-Methoxyethylamine	$CH_3OCH_2CH_2NH_2$	75.11	4^2, 718	0.864	1.4054^{20}		95	9	v s aq, alc
m78	2-Methoxyethyl cyanoacetate	$CH_3OCH_2CH_2O_2CCH_2CN$	143.14	2^4, 1891	1.127	1.4340^{20}		100^{1mm}	>110	
m79	1-Methoxy-2-indanol		164.20	6, 970	1.128	1.5482^{20}		146^{11mm}	>110	
m80	2-Methoxy-5-methyl-aniline	$CH_3OC_6H_3(CH_3)NH_2$	137.18	13^2, 388			52–54	235	>110	s aq; v s alc, bz, eth
m81	4-Methoxy-2-methyl-aniline	$CH_3OC_6H_3(CH_3)NH_2$	137.18	13^2, 330	1.065	1.5647^{20}	13–14	248–249	>110	s alc
m82	3-Methoxy-3-methyl-1-butanol	$CH_3OC(CH_3)_2CH_2CH_2OH$	118.18	1^3, 2198	0.926	1.4280^{20}		173–175	71	
m83	2-Methoxy-1-methyl-ethyl cyanoacetate	$NCCH_2CO_2CH(CH_3)CH_2OCH_3$	157.17		1.030	1.4310^{20}		105^{2mm}	62	
m84	2-Methoxy-4-methyl-phenol	$CH_3OC_6H_3(CH_3)OH$	138.17	6, 878	1.092	1.5372^{20}	5	222	99	
m85	5-Methoxy-2-methyl-4-nitroaniline	$CH_3OC_6H_3(CH_3)(NO_2)NH_2$	182.18	13^3, 1575			168–170			
m86	1-Methoxy-2-methyl-propylene oxide	$(CH_3)_2C(O)CH(OCH_3)$	102.13	17^3, 1035	0.904	1.3929^{20}		94	6	
m87	1-Methoxynaphthalene	$C_{10}H_7OCH_3$	158.20	6, 606	1.090	1.6220^{20}		135^{12mm}	>110	

Methoxyethane, e210

2-Methoxyethoxychloromethane, m74



m67



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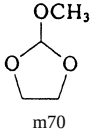
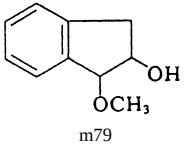


m70



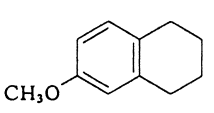
m79

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

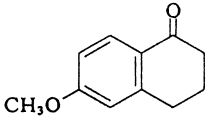
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
m88	2-Methoxynaphthalene	$C_{10}H_7OCH_3$	158.20	6, 640			73–75	274		s bz, eth, CS_2
m89	2-Methoxy-4-nitro-aniline	$CH_3OC_6H_3(NO_2)NH_2$	168.15	13, 390			140–142			
m90	2-Methoxy-5-nitro-aniline	$CH_3OC_6H_3(NO_2)NH_2$	168.15	13, 389			117–119			s alc, hot bz, HOAc
m91	4-Methoxy-2-nitro-aniline	$CH_3OC_6H_3(NO_2)NH_2$	168.15	13, 521			123–126			sl s aq; s alc, eth
m92	2-Methoxynitro-benzene	$CH_3OC_6H_4NO_2$	153.14	6, 217	1.2527_4^{20}	1.5161^{20}	10.5	277	>110	0.17 aq; s alc, eth
m93	4-Methoxy-3-nitro-benzoic acid	$CH_3OC_6H_3(NO_2)CO_2H$	197.15	10, 181			192–194			
m94	2-Methoxy-5-nitro-pyridine	$CH_3O(C_5H_3N)NO_2$	154.13	21^3, 33			108–109			
m95	4-Methoxy-2-nitro-toluene	$CH_3OC_6H_3(NO_2)CH_3$	167.16	6, 411	1.207	1.5525^{20}	17	267	>110	
m96	4-Methoxyphenethyl-amine	$CH_3OC_6H_3CH_2CH_2NH_2$	151.21	13, 626	1.033	1.5379^{20}		140^{20mm}	>110	
m97	2-Methoxyphenol	$CH_3OC_6H_4OH$	124.14	6, 768	1.112(lg)	1.5429	28	205	82	1.5 aq; misc alc, eth
m98	3-Methoxyphenol	$CH_3OC_6H_4OH$	124.14	6, 813	1.131	1.5510^{20}	< −17.5	115^{5mm}	>110	misc alc, eth; sl s aq
m99	4-Methoxyphenol	$CH_3OC_6H_4OH$	124.14	6, 843			55–57	243	>110	v s bz; s alk
m100	3-(4-Methoxy-phenoxy)-1,2-propanediol	$CH_3OC_6H_4OCH_2CH(OH)CH_2OH$	198.22	6^3, 4411			76–80			
m101	4-Methoxyphenyl-acetic acid	$CH_3OC_6H_4CH_2CO_2H$	166.18	10, 190			86–88	140^{3mm}		1 aq; v s alc; s eth
m102	2-Methoxyphenyl-acetone	$CH_3OC_6H_4CH_2OCH_3$	164.20	8^3, 397	1.054	1.5250^{20}		130^{10mm}	>110	s alc, eth
m103	2-(Methoxyphenyl)-acetonitrile	$CH_3OC_6H_4CH_2CN$	147.18	10, 188			65–68	143^{15mm}		s hot bz
m104	4-(Methoxyphenyl)-acetonitrile	$CH_3OC_6H_4CH_2CN$	147.18	10, 191	1.085	1.5300^{20}		286–287	>110	
m105	1-Methoxy-2-propanol	$CH_3OCH_2CH(OH)CH_3$	90.12	1^2, 536	0.919_{20}^{20}	1.4021^{21}	−97	120.1	33	misc aq, acet, bz, eth
m106	2-Methoxypropene	$CH_3C(OCH_3)=CH_2$	72.11	1, 435	0.735	1.3820^{20}		34–36	−29	

m107	*trans*-1-Methoxy-4-(1-propenyl)benzene	$CH_3OC_6H_4CH{=}CHCH_3$	148.21	6, 566	0.9883_4^{20}	1.5615^{20}	21.4	237	90	misc chl, eth; 50 alc; s bz, EtOAc
m108	2-Methoxy-4-propenylphenol	$CH_3OC_6H_3(OH)CH{=}CHCH_3$	164.20	6, 955	1.087_4^{20}	1.5748^{20}	−10	266	>112	misc alc, eth; sl s aq
m109	2-Methoxy-4-(2-propenyl)phenol	$CH_3OC_6H_3(OH)CH_2CH{=}CH_2$	164.20	6, 961	1.0664_4^{20}	1.5408^{20}	−9.2	255	>112	misc alc, chl, eth; s HOAc, alk; i aq
m110	3-Methoxypropionitrile	$CH_3OCH_2CH_2CN$	85.11	3[1], 113	0.937	1.4030^{20}		165	61	
m111	4-Methoxypropiophenone	$CH_3OC_6H_4COCH_2CH_3$	164.20	8, 103	1.071	1.5465^{20}	27–29	274	61	
m112	3-Methoxypropylamine	$CH_3O(CH_2)_3NH_2$	89.14	4[3], 739	0.874	1.4175^{20}		118^{733mm}	22	
m113	2-Methoxypyridine	$CH_3O(C_5H_4N)$	109.13	21, 44	1.038	1.5029^{29}		142	32	misc aq
m114	6-Methoxy-1,2,3,4-tetrahydronaphthalene		162.23	6[2], 537	1.033	1.5402^{20}		90^{1mm}	>110	
m115	6-Methoxy-1-tetralone		176.22	9[2], 889			77–79	171^{11mm}		
m116	2-Methoxytoluene	$CH_3OC_6H_4CH_3$	122.17	6, 352	0.9851_{15}^{15}	1.5161^{20}		170–172	51	i aq; v s alc, eth
m117	3-Methoxytoluene	$CH_3OC_6H_4CH_3$	122.17	6, 376	0.9697_{25}^{25}	1.5131^{20}		175–176	54	s alc, bz, eth; i aq
m118	4-Methoxytoluene	$CH_3OC_6H_4CH_3$	122.17	6, 392	0.969_{25}^{25}	1.5112^{20}		174	53	s alc, eth; i aq
m119	Methoxytrimethylsilane	$CH_3OSi(CH_3)_3$	104.23	4[3], 1856	0.7560_4^{20}	1.3678^{20}		57–58	−30	
m120	*N*-Methylacetamide	$CH_3CONHCH_3$	73.10	4, 58	0.9460^{35}	1.4253^{35}	30.6	206	108	s aq
m121	4′-Methylacetanilide	$CH_3OCONHC_6H_4CH_3$	149.19	12, 920			150	307		
m122	Methyl acetate	$CH_3CO_2CH_3$	74.08	2, 224	0.9342_4^{20}	1.3619^{20}	−98	57	−10 (CC)	24 aq; misc alc, eth
m123	Methyl acetoacetate	$CH_3COCH_2CO_2CH_3$	116.12	3, 632	1.0757^{20}	1.4186^{20}	27.5	171.7	77	50 aq; misc alc
m124	4′-Methylacetophenone	$CH_3C_6H_4COCH_3$	134.18	7, 307	1.0051	1.5328^{20}	22–24	226	92	i aq; v s alc, eth

α-Methoxy-α-phenylacetophenone, b49 3-Methoxypropionaldehyde dimethyl acetal, t341 6-Methoxytetralin, m114



m114



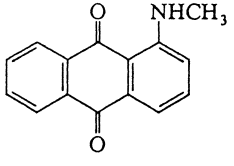
m115

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

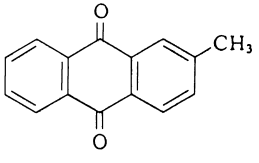
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
m125	Methyl 4-acetoxy-benzoate	$CH_3CO_2C_6H_4CO_2CH_3$	194.19	10, 159			82–84			
m126	Methyl acrylate	$H_2C{=}CHCO_2CH_3$	86.09	2, 399	0.9541_4^{20}	1.4040^{20}	−76.5	80.2	−3 (CC)	6 aq; s alc, eth
m127	Methylamine	CH_3NH_2	31.06	4, 32	0.699_4^{-11}		−93.5	−6.3	0	959 mL aq; 10.5 bz
m128	1-(Methylamino)-anthraquinone		237.26	14, 179			170–172			
m129	Methyl 2-amino-benzoate	$H_2NC_6H_4CO_2CH_3$	151.17	14, 317	1.168_4^{19}	1.5820^{20}	24	256	104	sl s aq; v s alc, eth
m130	Methyl 3-amino-crotonate	$CH_3C(NH_2){=}CHCO_2CH_3$	115.13	3, 632			81–83			
m131	2-(Methylamino)-ethanol	$CH_3NHCH_2CH_2OH$	75.11	4, 276	0.937^{20}	1.4387^{20}		159	72	misc aq, alc, eth
m132	4-Methylaminophenol sulfate	$(CH_3NC_6H_4OH)_2 \cdot H_2SO_4$	344.39	13, 441			260 dec			4 aq; sl s alc; i eth
m133	Methyl 2-(amino-sulfonyl)benzoate	$H_2HSO_2C_6H_4CO_2CH_3$	215.23	11, 377			126–128			
m134	*N*-Methylaniline	$C_6H_5NHCH_3$	107.16	12, 135	0.989_4^{20}	1.5684^{20}	−57	196	78	sl s aq; s alc, eth
m135	*N*-Methylanilinium trifluoroacetate	$C_6H_5NHCH_3 \cdot HO_2CCF_3$	221.18				65–66			
m136	2-Methyl-anthraquinone		222.24	7, 809			170–173			v s bz; s alc, eth
m137	Methylarsonic acid	$CH_3AsO(OH)_2$	139.96	4, 613			161			v s aq; s alc
m138	4-Methylbenzaldehyde	$CH_3C_6H_4CHO$	120.15	7, 297	1.0194_4^{17}	1.5447^{20}		205	80	misc alc, eth; sl s aq
m139	Methyl benzene-sulfonate	$C_6H_5SO_2OCH_3$	172.20	11^2, 20	1.2889_4^{0}	1.5151^{20}	−4	154^{20mm}		v s alc, chl, eth
m140	2-Methylbenzimida-zole		132.17	23, 145			176–177			s alk, hot aq; sl s alc
m141	Methyl benzoate	$C_6H_5CO_2CH_3$	136.15	9, 109	1.0933_4^{15}	1.5205^{15}	−15	199.5	83	0.2 aq; misc alc, eth
m142	2-Methylbenzoic acid	$CH_3C_6H_4CO_2H$	136.15	9, 462	1.062		103.7	258–259		sl s aq; v s alc
m143	3-Methylbenzoic acid	$CH_3C_6H_4CO_2H$	136.15	9, 475	1.054		111–113	263		0.09 aq; v s alc
m144	4-Methylbenzoic acid	$CH_3C_6H_4CO_2H$	136.15	9, 483			180	274–275		v s alc, eth
m145	4-Methylbenzo-phenone	$CH_3C_6H_4COC_6H_5$	196.25	7, 440			57	326		v s bz, eth
m146	2-Methylbenzothiazole		149.22	27, 46	1.173	1.6170^{20}	12–14	238	102	s alc, HOAc; i aq

m147	2-Methylbenzoxazole		133.15	27, 46	1.121	1.5497^{20}	8–10	178	75	
m148	α-Methylbenzyl acetate	$CH_3CO_2CH(CH_3)C_6H_5$	164.20	6, 476	1.028	1.4945^{20}		95^{12mm}	91	
m149	α-Methylbenzyl alcohol	$C_6H_5CH(CH_3)OH$	122.17	6, 475	1.0191^{13}_{4}	1.5265^{20}	20	204^{745mm}	85	v s alc; s bz, chl
m150	2-Methylbenzyl alcohol	$CH_3C_6H_4CH_2OH$	122.17	6, 484		1.5408^{20}	33–36	110^{14mm}	104	5 aq; 5 alc; s eth
m151	(±)-α-Methylbenzylamine	$C_6H_5CH(CH_3)NH_2$	121.18	12, 1094	0.940	1.5260^{20}		185	79	4.2 aq; misc alc, eth
m152	4-Methylbenzylamine	$CH_3C_6H_4CH_2NH_2$	121.18	12, 1141	0.952	1.5340^{20}	12–13	195	75	
m153	Methylbis(trimethylsilyloxy)vinyl ether	$CH_3Si[OSi(CH_3)_2]CH{=}CH_2$	148.55	4^4, 4184	0.864	1.3970^{20}		$48^{8.8mm}$	51	
m154	Methyl bromoacetate	$BrCH_2CO_2CH_3$	152.98	2, 213	1.616	1.4586^{20}		52^{15mm}	62	s alc
m155	(±)-Methyl 2-bromobutyrate	$CH_3CH_2CH(Br)CO_2CH_3$	181.04	2, 282	1.573	1.452^{20}		138^{50mm}	68	
m156	Methyl 2-bromopropionate	$CH_3CH(Br)CO_2CH_3$	167.01	2, 253	1.497	1.5420^{20}		51^{19mm}	51	s alc
m157	2-Methyl-1,3-butadiene	$H_2C{=}C(CH_3)CH{=}CH_2$	68.12	1, 252	0.681^{20}_{4}	1.4216^{20}	−146.0	34.1	−53	misc alc, eth

Methylal, d507
Methyl alcohol, m38
Methylallene, b448
Methylaminoacetaldehyde dimethyl acetal, d508
α-(1-Methylaminoethyl)benzyl alcohol, e2
Methylanilines, t180 thru t182
Methyl *o*-anisate, m304
Methyl *p*-anisate, m305
2-Methyl-*p*-anisidine, m80
5-Methyl-*o*-anisidine, m81
Methylanisoles, m116 thru m118
Methyl anthranilate, m129
Methylanthranilic acid, a207, a208
Methylbenzene, t166
4-Methylbenzenesulfonic acid, t176
Methyl benzilate, m239
2-Methylbenzonitrile, t184
4-Methylbenzonitrile, t185
o-Methylbenzyl alcohol, p109
N-Methylbenzylamine, b108
Methylbenzyl bromide, b343, b344
Methylbenzyl chlorides, c269 thru c271
Methylbis(2-chloroethoxy)silane, b162
N-Methylbis(2-chloroethyl)amine, b164
Methyl bromide, b225



m128



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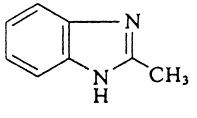
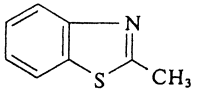
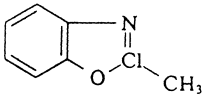


m140



m146



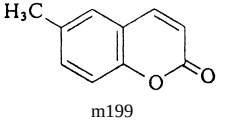
m147

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
m158	2-Methylbutane	$CH_3CH_2CH(CH_3)_2$	72.15	1, 134	0.6197^{20}	1.3537^{20}	−159.9	27.8	−56	0.005 aq; misc alc
m159	2-Methyl-1-butenethiol	$CH_3CH_2CH(CH_3)CH_2SH$	104.22	1^2, 421	0.848	1.4465^{20}		117	19	s alc, eth; i aq
m160	2-Methyl-2-butanethiol	$CH_3CH_2C(CH_3)_2SH$	104.22	1^1, 196	0.842	1.4385^{20}	−103.9	99.1	−1	s alc, eth; i aq
m161	2-Methyl-1-butanol	$CH_3CH_2CH(CH_3)CH_2OH$	88.15	1, 388	0.816_4^{20}	1.4100^{20}	< −70	128	43	3 aq; misc alc, eth
m162	2-Methyl-2-butanol	$CH_3CH_2C(CH_3)_2OH$	88.15	1, 388	0.8096^{20}	1.4050^{20}	−9.0	102.0	21	11 aq; misc alc, bz, chl, eth
m163	3-Methyl-1-butanol	$(CH_3)_2CHCH_2CH_2OH$	88.15	1, 392	0.8129_4^{15}	1.4085^{15}	−117	131	45	2 aq; misc alc, bz, chl, eth, PE, HOAc
m164	3-Methyl-2-butanol	$(CH_3)_2CHCH(OH)CH_3$	88.15	1, 391	0.8179^{20}	1.4091^{20}		112.9	38	2.8 aq; misc alc, eth
m165	3-Methyl-2-butanone	$(CH_3)_2CHCOCH_3$	86.13	1, 682	0.802_4^{20}	1.3880^{20}	−92	94.3	6	misc alc, eth
m165a	2-Methyl-1-butene	$C_2H_5C(CH_3)=CH_2$	70.14	1, 211	0.650	1.3780^{20}	−137.6	31	< −34	
m166	2-Methyl-2-butene	$CH_3CH=C(CH_3)_2$	70.14	1, 211	0.6620_4^{20}	1.3878^{20}	−133.8	38.6	−45	misc alc, eth; i aq
m167	3-Methyl-1-butene	$(CH_3)_2CHCH=CH_2$	70.14	1, 213	0.6272_4^{20}	1.3638^{20}	−168	20	−56	misc alc, eth
m168	*cis*-2-Methyl-2-butenoic acid	$CH_3CH=C(CH_3)CO_2H$	100.12	2, 428	0.983_4^{47}	1.4437^{47}	45	185		s alc, eth; v s hot aq
m169	*trans*-2-Methyl-2-butenoic acid	$CH_3CH=C(CH_3)CO_2H$	100.12	2, 430	0.969	1.4342^{81}	64	198		s alc, eth; v s hot aq
m170	3-Methyl-2-butenoic acid	$(CH_3)_2C=CHCO_2H$	100.12	2, 432	1.006^{24}		69	194–195		s aq, alc, eth
m171	2-Methyl-3-buten-2-ol	$(CH_3)_2C(OH)CH=CH_2$	86.13	1, 444	0.824	1.4170^{20}	2.6	98–99	13	
m172	3-Methyl-2-buten-1-ol	$(CH_3)_2C=CHCH_2OH$	86.13	1, 444	0.848	1.4440^{20}		140	43	
m173	3-Methyl-3-buten-1-ol	$H_2C=C(CH_3)CH_2CH_2OH$	86.13		0.853	1.4337^{20}			36	
m174	2-Methyl-1-buten-3-yne	$H_2C=C(CH_3)C\equiv CH$	66.10	1^1, 126	0.695	1.4140^{20}	−113	32	−6	
m175	*N*-Methylbutylamine	$CH_3CH_2CH_2CH_2NCH_3$	87.17	4, 157	0.736	1.3995^{20}	−75	91	1	
m176	1-Methylbutylamine	$CH_3CH_2CH_2CH(CH_3)NH_2$	87.17	4, 177	0.7384_4^{20}	1.4029^{20}		91	35	misc aq, alc, eth
m177	3-Methylbutyl 3-methylbutyrate	$(CH_3)_2CHCH_2CH_2O_2CCH_2$-$CH(CH_3)_2$	172.27	2, 312	0.8541^{25}	1.4100^{25}		190.4	84	misc alc, eth
m178	3-Methyl-1-butyne	$(CH_3)_2CHC\equiv CH$	68.12	1, 251	0.666_4^{20}	1.3740^{20}	−89.8	26.4		misc alc, eth
m179	2-Methyl-3-butyne-2-ol	$(CH_3)_2C(OH)C\equiv CH$	84.12	1^1, 235	0.8672_{20}^{20}	1.4209^{20}	2.6	104	25	misc aq, acet, bz
m180	2-Methylbutyraldehyde	$CH_3CH_2CH(CH_3)CHO$	86.13	1^1, 352	0.804	1.3919^{20}		90–92	4	
m181	3-Methylbutyraldehyde	$(CH_3)_2CHCH_2CHO$	86.13	1, 684	0.785_{20}^{20}	1.3882^{20}	−51	92–93	19	misc alc, eth; sl s aq
m182	Methyl butyrate	$CH_3CH_2CH_2CO_2CH_3$	102.13	2, 270	0.898_4^{20}	1.3860^{20}	−85.8	103	11	1.4 aq; misc alc, eth
m183	2-Methylbutyric acid	$CH_3CH_2CH(CH_3)CO_2H$	102.13	2, 305	1.4055^{20}			176.5	73	

m184	3-Methylbutyric acid	$(CH_3)_2CHCH_2CO_2H$	102.13	2, 309	0.9308_4^{20}	1.4033^{20}	−29.3	176.5	70	4 aq; s alc, chl, eth
m185	3-Methylbutyronitrile	$(CH_3)_2CHCH_2CN$	83.13	2^2, 278	0.7925_4^{19}	1.3927^{20}	−101	129		misc alc, eth
m186	3-Methylbutyryl chloride	$(CH_3)_2CHCH_2COCl$	120.58	2, 315	0.985_4^{20}	1.4161^{20}		115–117	18	dec aq, alc; s eth
m187	Methyl carbamate	$H_2NCO_2CH_3$	75.07	3, 21	1.136_4^{56}		56–58	177		220 aq; 73 alc; s eth
m188	Methyl chloroacetate	$ClCH_2CO_2CH_3$	108.52	2, 197	1.238_{20}^{20}	1.4220^{20}	−32	130	51	i aq; misc alc, eth
m189	Methyl 2-chloroaceto-acetate	$CH_3COCH(Cl)CO_2CH_3$	150.56		1.236	1.4465^{20}	−32.7	137	71	
m190	Methyl 4-chloroaceto-acetate	$ClCH_2COCH_2CO_2CH_3$	150.56	3^2, 426	1.305	1.4564^{20}		85^{4mm}	102	
m191	Methyl 3-chloro-benzoate	$ClC_6H_4CO_2CH_3$	170.60	9, 338	1.227	1.4923^{20}	21	101^{12mm}	104	
m192	Methyl-4-chloro-benzoate	$ClC_6H_4CO_2CH_3$	170.60	9, 340	1.382^{20}		42–44		106	s alc
m193	Methyl 4-chloro-butyrate	$ClCH_2CH_2CH_2CO_2CH_3$	136.58	2, 278	1.1268^{14}	1.4321^{20}		175–176	59	v s eth; s alc, acet
m194	Methyl chloroformate	$ClCO_2CH_3$	94.50	3, 9	1.223_4^{20}	1.3865^{20}		70–72	17	misc alc, bz, chl, eth
m195	Methyl 3-(chloro-formyl)propionate	$CH_3O_2CCH_2CH_2COCl$	150.56	2^2, 553	1.223	1.4402^{20}		65^{3mm}	73	
m196	Methyl 2-chloro-propionate	$CH_3CH(Cl)CO_2CH_3$	122.55	2, 248	1.075	1.4193^{20}		132–133	38	s alc
m197	2-Methylcinnam-aldehyde	$C_6H_5CH{=}C(CH_3)CHO$	146.19	7, 369	1.0407_4^{17}	1.6045^{20}		149^{27mm}	79	
m198	Methyl *trans*-cinnamate	$C_6H_5CH{=}CHCO_2CH_3$	162.19	9, 581			36–38	262	>110	
m199	6-Methylcoumarin		160.17	17, 337			75–76	303^{725mm}		

3-Methyl-1-butencarboxylic acid, m369
cis-2-Methyl-2-butenedioic acid, c284
Methyl 2-buten-1-oate, m200
3-Methylbutyl acetate, i91
2-Methylbutylamine, a246
Methyl *tert*-butyl ether, b572
2-Methylbutyl isovalerate, m177
Methyl *tert*-butyl ketone, h70
Methyl caprate, m226
Methyl caproate, m270
Methyl caprylate, m349
Methyl carbazate, m275
Methyl carbitol, m73
4-Methylcatechol, d438
Methyl cellosolve, m71
Methyl cellosolve acetate, m75
Methyl chlorocarbonate, m194
Methyl chloroform, t231



m199

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

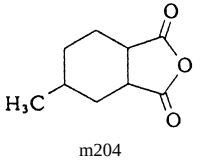
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
m200	Methyl crotonate	$CH_3CH{=}CHCO_2CH_3$	100.12	2, 410	0.9444_4^{20}	1.4242^{20}		121	4	v s alc, eth; i aq
m201	Methyl cyanoacetate	$NCCH_2CO_2CH_3$	99.09	2, 584	1.1225^{25}	1.4166^{25}	−22.5	201	>110	misc alc, eth
m202	Methylcyclohexane	$C_6H_{11}CH_3$	98.19	5, 29	0.7694^{20}	1.4221^{20}	−126.6	100.9	−4	
m203	Methyl cyclohexane-carboxylate	$C_6H_{11}CO_2CH_3$	142.20	9, 8	0.9954_4^{16}	1.4430^{20}		183	60	i aq; s alc, eth
m204	4-Methyl-1,2-cyclo-hexanedicarboxylic anhydride		168.19		1.162	1.4774^{20}			>110	
m205	1-Methylcyclohexanol	$CH_3C_6H_{10}OH$	114.19	6, 11	0.9251^{25}	1.4587^{25}	25	155	67	i aq; b bz, chl
m206	*cis*-2-Methylcyclo-hexanol	$CH_3C_6H_{10}OH$	114.19	6[2], 17	0.9360_4^{20}	1.4640^{30}	7	165	58	misc alc, eth
m207	*trans*-2-Methylcyclo-hexanol	$CH_3C_6H_{10}OH$	114.19	6, 11	0.9247_4^{20}	1.4616^{20}	−2	167.5	65	misc alc; s eth
m208	*cis*-3-Methylcyclo-hexanol	$CH_3C_6H_{10}OH$	114.19	6, 12	0.9155^{20}	1.4572^{20}	−6	168	62	misc alc, eth
m209	*trans*-3-Methylcyclo-hexanol	$CH_3C_6H_{10}OH$	114.19	6, 12	0.9214^{20}	1.4580^{20}	−0.5	167	62	
m210	*cis*-4-Methylcyclo-hexanol	$CH_3C_6H_{10}OH$	114.19	6, 14	0.9170^{20}	1.4614^{20}	−9.2	173	70	misc alc, eth
m211	*trans*-4-Methylcyclo-hexanol	$CH_3C_6H_{10}OH$	114.19	6, 14	0.9118_4^{21}	1.4559^{20}		174	70	misc alc; s eth
m212	2-Methylcyclo-hexanone	$CH_3C_6H_9(=O)$	112.17	7, 14	0.925_4^{20}	1.4478^{20}		162	46 (CC)	i aq; s alc, eth
m213	3-Methylcyclo-hexanone	$CH_3C_6H_9(=O)$	112.17	7, 15	0.9155_4^{20}	1.4460^{20}		169	51	i aq; s alc, eth
m214	4-Methylcyclo-hexanone	$CH_3C_6H_9(=O)$	112.17	7, 18	0.916_4^{20}	1.4455^{20}		171	40	i aq; s alc, eth
m215	1-Methyl-1-cyclo-hexene		96.17	5, 66	0.809_4^{20}	1.4502^{20}	−121	111	−3	i aq; s alc, eth
m216	4-Methyl-1-cyclo-hexene		96.17	5, 67	0.799	1.4412^{20}	−115.5	102	−1	i aq; s alc, eth
m217	6-Methyl-3-cyclo-hexene-1-methanol		126.20		0.954	1.4830^{20}				

m218	*N*-Methylcyclohexylamine	$C_6H_{11}NHCH_3$	113.20	12, 6	0.868	1.4560^{20}		149	29	
m219	3-Methylcyclohexylamine	$CH_3C_6H_{10}NH_2$	113.20	12, 10	0.855	1.4525^{20}		150^{730mm}	22	
m220	4-Methylcyclohexylamine	$CH_3C_6H_{10}NH_2$	113.20	12, 12	0.955	1.4531^{20}		151–154	26	
m221	Methylcyclopentadiene dimer		160.26	5^4, 1435	0.941	1.4976^{20}	−51	200	26	
m222	Methylcyclopentane	$C_5H_9CH_3$	84.16	5, 27	0.7487^{20}	1.4097^{20}	−142.4	71.8	−23	0.013 aq
m223	3-Methyl-1,2-cyclopentanedione		112.13	7^1, 310			105–107			
m224	2-Methylcyclopentanone		98.15	7^2, 13	0.9200_4^{20}	1.4347^{20}	−76	139	26	s aq; v s alc, eth
m225	Methyl cyclopropanecarboxylate	$C_3H_5CO_2CH_3$	100.12	9^1, 3	0.985	1.4181^{20}		119	17	
m226	Methyl decanoate	$CH_3(CH_2)_8CO_2CH_3$	186.30	2, 356	0.873	1.4255^{20}	−18	223	94	i aq; misc alc, eth
m227	Methyl dichloroacetate	$Cl_2CHCO_2CH_3$	142.97	2, 203	1.3808^{19}	1.4421^{20}	−52	143	80	i aq; s alc
m228	Methyl 2,2-dichloro-1-methylcyclopropanecarboxylate		183.03		1.245	1.4639^{20}		74^{8mm}	74	
m229	Methyl 2,3-dichloropropionate	$ClCH_2CH(Cl)CO_2CH_3$	157.00	2^1, 111	1.3282_4^{20}	1.4447^{20}		92^{50mm}	42	s alc
m230	*N*-Methyldiethanolamine	$CH_3N(CH_2CH_2OH)_2$	119.16	4, 284	1.0377^{20}	1.4685^{20}		248	126	misc aq, alc
m231	Methyl 3,4-dimethoxybenzoate	$(CH_3O)_2C_6H_3CO_2CH_3$	196.20	10, 396			59–62	283		
m232	Methyl 3,5-dimethoxybenzoate	$(CH_3O)_2C_6H_3CO_2CH_3$	196.20	10, 405			43	298	>110	

trans-2-Methylcrotonic acid, m169

Methyl cyanide, a29

Methyl 4,6-dimethyl-2-oxo-2*H*-pyran-5-carboxylate, m292



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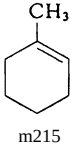

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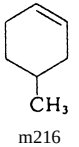

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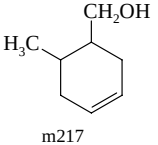

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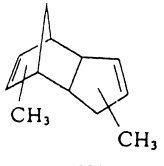

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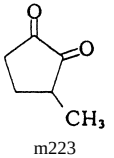

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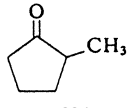

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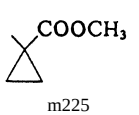

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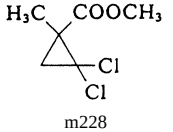


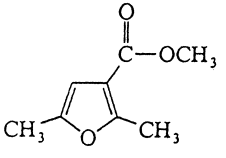
m228

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
m233	Methyl 3-(dimethylamino)propionate	$(CH_3)_2NCH_2CH_2CO_2CH_3$	131.18	4, 403	0.917	1.4184^{20}		154	51	
m234	Methyl 2,5-dimethyl-3-furoate		154.17	18, 398	1.037	1.4750^{20}		198	80	
m235	Methyl 2,2-dimethylpropionate	$(CH_3)_3CCO_2CH_3$	116.16	2^1, 139	0.873	1.3880^{20}		101–103	−1	misc alc, eth; sl s aq
m236	*N*-Methyldioctylamine	$(C_8H_{17})_2NCH_3$	255.49	4^3, 381	1.066	1.4424^{20}	−30.1	165^{15mm}	>110	
m237	4-Methyl-1,3-dioxane		102.13	19^4, 49	0.976	1.4150^{20}	−45	114	22	
m238	*N*-Methyldiphenylamine	$(C_6H_5)_2NCH_3$	183.26	12, 180	1.048_4^{20}	1.6193^{20}	−7.6	135^{6mm}		i aq; s alc, eth
m239	Methyl diphenylglycolate	$(C_6H_5)_2C(OH)CO_2CH_3$	242.27	10, 344			74–76	187^{13mm}		
m240	3-Methyl-1,1-diphenylurea	$(C_6H_5)_2NCONHCH_3$	226.28	12,*2*, 852			172–174			
m241	Methyleneaminoacetonitrile	$CH_2{=}NCH_2CN$	68.08	Merck: 11, 5976			129			s hot aq, alc; sl s bz
m242	*N*,*N*′-Methylenebisacrylamide	$H_2C{=}CHC(=O)NHCH_2NHC(=O)CH{=}CH_2$	154.17				>300			
m243	2,2′-Methylenebis(4-chlorophenol)	$CH_2[C_6H_3(Cl)OH]_2$	269.13	6,*3*, 5408			168–172			100 EtOH; 100 eth; s PE
m244	4,4′-Methylenebis(2,6-di-*tert*-butylphenol	$CH_2\{C_6H_2[C(CH_3)_3]_2OH\}_2$	424.67	6^4, 6811			156–158	289^{40mm}		
m245	4,4′-Methylenebis(*N*,*N*-dimethylaniline)	$CH_2[C_6H_4N(CH_3)_2]_2$	254.38	13, 239			88–89			
m246	1,1′-Methylenebis(3-methylpiperidine)	$CH_2[CH_3C_5H_9N]_2$	210.37		0.887	1.4734^{20}		160^{50mm}	>110	
m247	4,4′-Methylenebis(phenylisocyanate)	$CH_2(C_6H_4NCO)_2$	250.26	13,*3*, 461	1.180		42–44	200^{5mm}	>110	
m248	Methylene blue		373.90	27, 393			190 dec			4 aq; 1.3 alc; s chl
m249	4,4′-Methylenedianiline	$CH_2(C_6H_4NH_2)_2$	198.26	13, 238			89–91	399	221	v s alc, bz, eth; sl s aq

m250	3,4-Methylenedioxybenzaldehyde		150.13	19, 115			37	264	>110	0.2 aq; v s alc, eth
m251	1,2-Methylenedioxybenzene		122.12	19, 20	1.064	1.5398		173	55	
m252	3,4-Methylenedioxy-6-propylbenzyldiethyleneglycol butyl ether		338.45	19[3], 779	1.059	1.498		180[1mm]	171	misc alc, bz, geons
m253	Methylenesuccinic acid	$H_2C{=}C(CO_2H)CH_2CO_2H$	130.10	2, 760	1.573		167			8.2 aq; 20 alc; v sl s bz, chl, eth, PE

Methyldinitrophenol, d715, d716
Methyl enanthate, m266
Methylene bromide, d110
Methylene bromochloride, b305
Methylene chloride, d235
4,4′-Methylenedianiline, d46
Methylene dimethyl ether, d507
1,1′-Methylenedipiperidine, d776
Methylene fluoride, d409
Methylene iodide, d452
β-Methylene-β-propiolactone, d483
(1-Methylethyl)benzene, i103
Methyl ethyl ketone, b475



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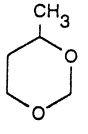

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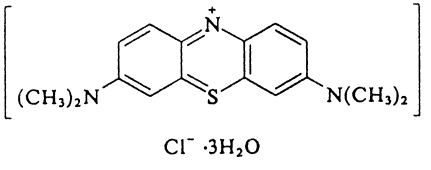

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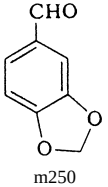

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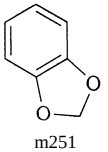

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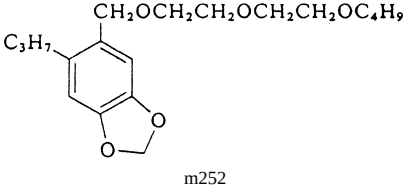


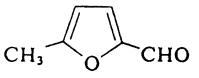
m252

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
m254	*N*-Methylethylene-diamine	$CH_3NHCH_2CH_2NH_2$	74.13	4^1, 415	0.841	1.4395^{20}		114–116	42	
m255	*N*-Methylformamide	$HC(=O)NHCH_3$	59.07	4, 58	0.9988^{25}	1.4300^{25}	−4	199.5	98	misc aq
m256	*N*-Methylformanilide	$C_6H_5N(CH_3)CHO$	135.17	12, 234	1.095	1.5610^{20}	8–13	244	126	
m257	Methyl formate	HCO_2CH_3	60.05	2, 18	0.9815^{15}	1.3465^{15}	−99	31.7	−19	30 aq; misc alc
m258	5-Methylfuraldehyde		110.11	17, 289	1.1072_4^{18}	1.5263^{20}		187	72	s aq; v s alc; misc eth
m259	2-Methylfuran		82.10	17, 36	0.915_4^{20}	1.4332^{20}	−88	63–66	−22	0.3 aq
m259a	Methyl 2-furoate		126.11	18, 274	1.179^{20}	1.4879^{20}		181	73	s alc, eth; sl s aq
m260	Methylgermanium tribromide	CH_3GeBr_3	327.35		2.6337_4^{20}	1.5770^{20}		168		
m261	*N*-Methylglucamine		195.22	Merck: 12, 6154			128–129			100 aq^{25}; 1.2 alc^{70}
m262	Methyl-α-**D**-gluco-pyranoside		194.18	31, 179	1.46_4^{30}		168	$200^{0.2mm}$		63 aq; 1.6 alc; i eth
m263	(±)-2-Methylglutaro-nitrile	$NCCH_2CH_2CH(CH_3)CN$	108.14	2, 656	0.950	1.4340^{20}	−45	269–271	126	
m264	*N*-Methylglycine	$CH_3NHCH_2CO_2H$	89.09	4, 345			208 dec			42 aq; sl s alc
m265	Methyl glycolate	$HOCH_2CO_2CH_3$	90.08	3, 236	1.168_4^{18}	1.4170^{20}	74	151	67	s aq; misc alc, eth
m266	Methyl heptanoate	$CH_3(CH_2)_5CO_2CH_3$	144.22	2, 339	0.8815_4^{20}	1.4115^{20}	−55.8	173.5	52	s alc, eth; sl s aq
m267	5-Methyl-2-heptanol	$(CH_3)_2CH(CH_2)_3CH(OH)CH_3$	130.23	1, 421	0.803	1.4240^{20}		172	67	
m268	5-Methyl-3-heptanone	$C_2H_5CH(CH_3)CH_2COC_2H_5$	128.22	1^1, 363	0.823	1.4142^{20}		157–162	43	
m269	6-Methyl-5-hepten-2-one	$(CH_3)_2C{=}CHCH_2CH_2COCH_3$	126.20	1^3, 3010	0.855_4^{16}	1.4392^{20}	−67	73^{18mm}	50	misc alc, eth
m269a	Methyl hexadecanoate	$CH_3(CH_2)_{14}CO_2CH_3$	270.46	2, 372	0.852	1.4512^{20}	32–34	196^{15mm}	>110	s alc, chl, eth
m270	Methyl hexanoate	$CH_3(CH_2)_4CO_2CH_3$	130.19	2, 323	0.9038_4^0	1.4038^{23}	−71	151	45	v s alc, eth
m271	5-Methyl-2-hexanone	$(CH_3)_2CHCH_2CH_2COCH_3$	114.19	1^2, 756	0.888_4^{20}	1.4062^{20}	−73.9	144	3641	0.5 aq; misc alc, eth
m272	1-Methylhexylamine	$CH_3(CH_2)_4CH(NH_2)CH_3$	115.22	4, 194	0.7665^{18}	1.4175^{20}		144	54	sl s aq; s alc, eth
m273	1-Methylhydantoin		114.10	24, 244			157	subl		s aq, alc; 3 eth
m274	Methylhydrazine	CH_3NHNH_2	46.07	4^2, 957	0.866	1.4225^{20}	−52.4	87.5	21	misc aq, alc; s PE
m275	Methyl hydrazino-carboxylate	$H_2NNHCO_2CH_3$	90.08	3^1, 46			70–73	108^{12mm}		
m276	Methyl hydrogen glutarate	$HO_2CCH_2CH_2CH_2CO_2CH_3$	146.14	2^2, 565	1.169	1.4381^{20}		151^{10mm}	>110	

m277	Methyl hydrogen hexanedioate	$HO_2C(CH_2)_4CO_2H$	160.17	2, 652	1.081	1.4401^{20}	8–9	162^{10mm}	>110	s alc
m278	Methyl hydrogen succinate	$HO_2CCH_2CH_2CO_2H$	132.12	2, 608			56–59	151^{20mm}		v s aq, alc, eth
m279	Methyl hydroperoxide	CH_3OOH	48.04	1^2, 270	1.997_4^{15}	1.3642^{15}		38^{65mm}		misc aq, alc, eth; s bz
m280	Methylhydroquinone	$CH_3C_6H_3$—1,4-$(OH)_2$	124.14	6, 874			128–130			
m281	Methyl 4-hydroxybenzoate	$HOC_6H_4CO_2CH_3$	152.15	10, 158			126–128	270 dec		v s alc, eth, acet; 0.25 aq
m282	Methyl 2-hydroxyisobutyrate	$(CH_3)_2C(OH)CO_2CH_3$	118.13	3^2, 223	1.023	1.4112^{20}		127	42	v s aq, alc
m283	Methyl 4-hydroxyphenylacetate	$HOC_6H_4CH_2CO_2CH_3$	166.18	10, 191			57–60	163^{5mm}		
m284	2-Methylimidazole		82.11	23, 46	1.030	1.4960^{20}	−60	198	92	misc aq
m285	2-Methylimidazole		82.11	23, 65			142–143	268		

Methyl 2-furancarboxylate, m259a
5-Methylfurfural, m258
Methyl gallate, m454
α-Methyl-**D**-glucopyranoside, m262
N-Methylguanidine acetic acid, c301
4-Methylhexahydrophthalic anhydride, m204
Methyl hydroxyacetate, m265
Methyl 2-hydroxypropionate, m296
2,2′-Methyliminodiethanol, m230
2,2′-Methyliminobis(acetaldehyde diethyl acetal), b176
Methyl iodide, i37
Methyl isoamyl ketone, m271
Methyl isobutenyl ketone, m370
Methyl isobutyl ketone, m367
Methyl isonicotinate, m413
Methyl isopentyl ketone, m271
2-Methyllactic acid, h138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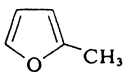
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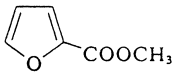
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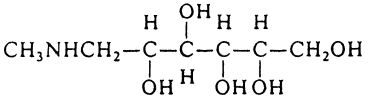
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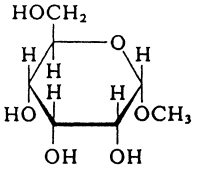
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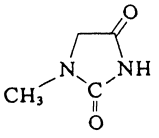
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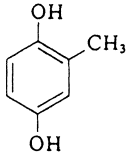
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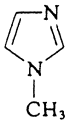
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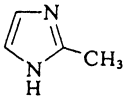
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TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

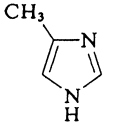
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
m286	4-Methylimidazole		82.11	23, 69			53–56	263	>110	
m287	2-Methyl-1*H*-indole		131.18	20, 311	1.07_4^{20}		58–60	273		v s alc, eth; s hot aq
m288	2-Methylindoline		133.19	20, 279	1.023	1.5681^{20}		229	93	
m289	*N*-Methylisatoic anhydride		177.16	27, 265			165 dec			
m290	Methyl isobutyrate	$(CH_3)_2CHCO_2CH_3$	102.13	2, 290	0.891^{20}	1.3840^{20}	−84.7	92.5	3	misc alc, eth; sl s aq
m291	Methyl isocyanate	CH_3NCO	57.05	4, 77	0.967	1.3695^{20}	−45	39	−6	s aq
m292	Methyl isodehydracetate		182.18	18, 410			68–70	167^{14mm}		
m293	*N*-Methylisopropylamine	$(CH_3)_2CHNHCH_3$	73.14	4[1], 153	0.702	1.3840^{20}	50–53		−31	
m294	Methyl isothiocyanate	CH_3NCS	73.12	4, 77	1.069	1.5258^{37}	35	118	32	v s alc, eth; sl s aq
m295	5-Methylisoxazole		83.09	27, 16	1.018	1.4386^{20}		122	30	
m296	Methyl lactate	$CH_3CH(OH)CO_2CH_3$	104.10	3, 280	1.088_4^{20}	1.4131^{20}		144–145	49	s aq (dec), alc, eth
m297	Methyl mandelate	$C_6H_5CH(OH)CO_2CH_3$	166.18	10, 202	1.1756^{20}		54–56	135^{12mm}	>110	s aq, alc, bz, chl
m298	Methyl mercaptoacetate	$HSCH_2CO_2CH_3$	106.14		1.187	1.4657^{20}		43^{10mm}	30	s alc, eth
m299	Methyl 3-mercaptopropionate	$HSCH_2CH_2CO_2CH_3$	120.17	3[2], 214	1.085	1.4660^{20}		55^{14mm}	60	
m300	Methyl methacrylate	$H_2C{=}C(CH_3)CO_2CH_3$	100.12	2[2], 398	0.9433^{20}	1.4140^{20}	−48	100	10	1,6 aq; s ketones, esters, CCl_4
m301	Methyl methanesulfonate	$CH_3SO_2OCH_3$	110.13	4, 4	1.2943_4^{20}	1.4138^{20}		202–203	104	20 aq; 100 DMF
m302	Methyl methoxyacetate	$CH_3OCH_2CO_2CH_3$	104.11	3, 236	1.0511_4^{20}	1.3964^{20}		130	35	v s alc, eth; sl s aq
m303	Methyl 4-methoxyacetoacetate	$CH_3OCH_2COCH_2CO_2CH_3$	146.14	3[4], 1939	1.129	1.4316^{20}		$89^{8.5mm}$	89	
m304	Methyl 2-methoxybenzoate	$CH_3OC_6H_4CO_2CH_3$	166.18	10, 71	1.157	1.5335^{20}		248	>110	
m305	Methyl 4-methoxybenzoate	$CH_3OC_6H_4CO_2CH_3$	166.18	10, 159			51	245	>110	
m306	Methyl 4-methoxyphenylacetate	$CH_3OC_6H_4CH_2CO_2CH_3$	180.20	10, 191	1.135	1.5165^{20}		158^{19mm}	36	
m307	Methyl 4-methoxypropionate	$CH_3OCH_2CH_2CO_2CH_3$	118.13	3, 297	1.009	1.4020		142–143	47	

m308	1-Methyl-4-(methylamino)piperidine		128.22		0.882	1.4672^{20}			55	
m309	Methyl 2-methylbenzoate	$CH_3C_6H_4CO_2CH_3$	150.18	9, 463	1.073	1.5190^{20}		207–208	82	
m310	Methyl 3-methylbenzoate	$CH_3C_6H_4CO_2CH_3$	150.18	9, 475	1.063	1.5160^{20}		113^{27mm}	95	
m311	Methyl 4-methylbenzoate	$CH_3C_6H_4CO_2CH_3$	150.18	9, 484			33–36	104^{15mm}	90	
m312	Methyl 2-methylbutyrate	$C_2H_5CH(CH_3)CO_2CH_3$	116.16	2, 304	0.885	1.3931^{20}		115	32	sl s aq; misc alc, eth
m313	2-Methyl-6-methylene-2-octanol	$C_2H_5C(=CH_2)(CH_2)_3C(CH_3)_2OH$	156.27		0.784	1.4431^{20}		84^{10mm}	76	
m314	Methyl 2-methyl-3-furancarboxylate		140.14		1.116	1.4730^{20}		75^{20mm}	63	

Methyl mercaptan, m37
Methylmercaptoanilines, m436
4-Methylmercaptobenzaldehyde, m437

2-Methyl-2-methoxypropane, b572
7-Methyl-3-methylene-1,6-octadiene, m467
1-Methyl-4-(1-methylethenyl)cyclohexane, d736

5-Methyl-2-(1-methylethyl)cyclohexanol, m12
5-Methyl-2-(1-methylethyl)cyclohexanone, m13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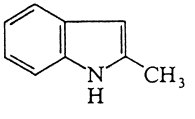
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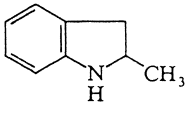
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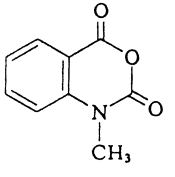
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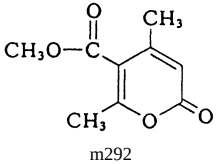
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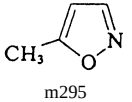
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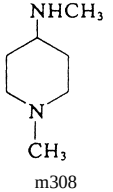
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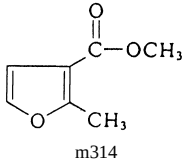
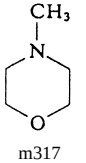

m314

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
m315	Methyl *S*-methylthio-methyl sulfoxide	$CH_3S(=O)CH_2SCH_3$	124.22		1.191	1.5487^{20}		$95^{2.5mm}$	>110	
m316	Methyl 3-(methyl-thio)propionate	$CH_3SCH_2CH_2CO_2CH_3$	134.20		1.077	1.4650^{20}		75^{13mm}	72	
m317	4-Methylmorpholine		101.15	27, 6	0.920	1.4349^{20}	−66	116	23	s aq, alc, eth
m318	1-Methylnaphthalene	$C_{10}H_7CH_3$	142.20	5, 566	1.0202^{20}	1.6170^{20}	−30.4	245	82	v s alc, eth
m319	2-Methylnaphthalene	$C_{10}H_7CH_3$	142.20	5, 567	1.029_4^{20}	1.6026^{40}	34.4	241	97	v s alc, eth
m320	Methyl 1-naphthalene-acetate	$C_{10}H_7CH_2CO_2CH_3$	200.24	9[3], 3206	1.142	1.5961^{20}		162^{5mm}	>110	
m321	2-Methyl-1,4-naphtho-quinone		172.18	7[2], 656			105–107			1.4 alc; 10 bz; s chl
m322	Methyl 1-naphthyl ketone	$C_{10}H_7COCH_3$	170.21	7, 401	1.1336_4^0	1.6284^{20}	11	302	>110	s alc, eth; i aq
m323	Methyl 2-naphthyl ketone	$C_{10}H_7COCH_3$	170.21	7, 402			53–55	301	>110	sl s alc; s CS_2
m324	Methyl nitrate	CH_3ONO_2	77.04	1, 284	1.2075_4^{20}	1.3748^{20}	−83	64 expl		sl s aq; s alc, eth
m325	Methyl nitrite	CH_3ONO	61.04	1, 284	0.991(lq)			−17.3		s alc, eth
m326	*N*-Methyl-4-nitro-aniline	$O_2NC_6H_4NHCH_3$	152.15	12, 714			152–154			
m327	2-Methyl-3-nitro-aniline	$CH_3C_6H_3(NO_2)NH_2$	152.15	12, 848			88–90	305		
m328	2-Methyl-4-nitro-aniline	$CH_3C_6H_3(NO_2)NH_2$	152.15	12, 846	1.1586_4^{140}		131–133			v s alc; s bz
m329	2-Methyl-5-nitro-aniline	$CH_3C_6H_3(NO_2)NH_2$	152.15	12, 844			104–107			s alc, acet, eth
m330	4-Methyl-2-nitro-aniline	$CH_3C_6H_3(NO_2)NH_2$	152.15	12, 1000			115–116			v s alc; s eth
m331	Methyl 2-nitro-benzoate	$O_2NC_6H_4CO_2CH_3$	181.15	9, 372	1.280	1.5340^{20}	−13	$106^{0.1mm}$	>110	s alc, eth
m332	Methyl 3-nitro-benzoate	$O_2NC_6H_4CO_2CH_3$	181.15	9, 378			78–80	279		
m333	Methyl 4-nitro-benzoate	$O_2NC_6H_4CO_2CH_3$	181.15	9, 390			94–96			

m334	2-Methyl-3-nitro-benzoic acid	$CH_3C_6H_3(NO_2)CO_2H$	181.15	9, 471			182–184			
m335	3-Methyl-4-nitro-benzoic acid	$CH_3C_6H_3(NO_2)CO_2H$	181.15	9, 481			216–218			
m336	4-Methyl-3-nitro-benzoic acid	$CH_3C_6H_3(NO_2)CO_2H$	181.15	9, 502			187–190			
m337	5-Methyl-2-nitro-benzoic acid	$CH_3C_6H_3(NO_2)CO_2H$	181.15	9, 482			134–136			
m338	2-Methyl-5-nitro-imidazole		127.10	23^{1}, 23			252–254			
m339	3-Methyl-4-nitro-phenol	$CH_3C_6H_3(NO_2)OH$	153.14	6, 386			127–129			
m340	4-Methyl-2-nitro-phenol	$CH_3C_6H_3(NO_2)OH$	153.14	6, 412	1.240_4^{40}	1.574^{40}	32–35	125^{22mm}	108	v s alc, eth
m341	2-Methyl-2-nitro-1-propanol	$O_2NC(CH_3)_2CH_2OH$	119.12	1, 378			86–89	95^{10mm}		350 aq
m342	2-Methyl-2-nitropropyl methacrylate	$H_2C{=}C(CH_3)CO_2CH_2$-$C(CH_3)_2NO_2$	187.20	2^{3}, 1288	1.087	1.4500^{20}		102^{4mm}	>110	
m343	*N*-Methyl-*N*-nitroso-4-toluenesulfonamide	$CH_3C_6H_4SO_2N(CH_3)NO$	214.24	11^{1}, 29			62			
m344	Methyl 2-nonynoate	$CH_3(CH_2)_5C{\equiv}CCO_2CH_3$	168.24	2, 490	0.915	1.4484^{20}		121^{20mm}	100	
m345	Methyl-5-norbornene-2,3-dicarboxylic anhydride		178.19	17^{2}, 461	1.232	1.5060^{20}			>110	
m346	Methyl octadecanoate	$CH_3(CH_2)_{16}CO_2CH_3$	298.51	2, 379			38	215^{15mm}	>110	s alc, eth

Methyl 2-methyllactate, m282
Methyl methyl-2-propenoate, m290
Methyl methylsulfinylmethyl sulfide, m315
Methyl myristate, m428
Methyl nicotinate, m412
4-Methyl-3-nitroanisol, m95
Methyl nonyl ketone, u9



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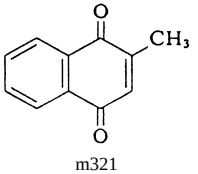

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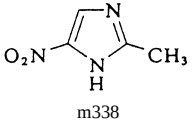

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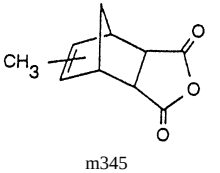


m345

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

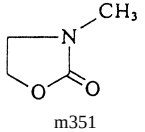
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
m347	Methyl *cis*-9-octadecenoate	$CH_3(CH_2)_7CH{=}CH(CH_2)_7CO_2CH_3$	296.50	2, 467	0.839^{20}	1.4521^{20}	−19.9	168^{2mm}	>110	misc abs alc, eth
m348	7-Methyl-1,6-octadiene	$(CH_3)_2C{=}CH(CH_2)_3CH{=}CH_2$	124.23	1^4, 1049	0.753	1.4360^{20}		143–144	26	
m349	Methyl octanoate	$CH_3(CH_2)_6CO_2CH_3$	158.24	2, 348	0.8775_4^{20}	1.4160^{25}	−40	192.9	72	v s alc, eth; i aq
m350	Methyl 2-octynoate	$CH_3(CH_2)_4C{\equiv}CCO_2CH_3$	154.21	2, 487	0.920	1.4460^{20}		217–220	88	
m351	3-Methyl-2-oxazolidinone		101.11		1.170	1.4541^{20}	15	90^{1mm}	>110	
m352	2-Methyl-2-oxazoline		85.11	27, 13	1.005	1.4340^{20}		110	20	
m353	3-Methyl-3-oxetanemethanol		102.13	17^3, 1128	1.024	1.4460^{20}		80^{40mm}	98	
m354	Methyl 2-oxocyclopentanecarboxylate	$(O{=})C_5H_7CO_2CH_3$	142.16	10, 597	1.145	1.4560^{20}		105^{19mm}	>110	
m355	Methyl 2-oxopropionate	$CH_3C(=O)CO_2CH_3$	102.09	3, 616	1.130	1.4065^{20}		134–137	39	misc alc, eth; sl s aq
m356	*trans*-2-Methyl-1,3-pentadiene	$CH_3CH{=}CHC(CH_3){=}CH_2$	82.15	1, 255	0.718	1.4469^{20}		75–76	−12	
m357	2-Methylpentane	$CH_3CH_2CH_2CH(CH_3)_2$	86.18	1, 148	0.6532^{20}	1.3725^{20}	−154	60.3	<−29	
m358	3-Methylpentane	$(CH_3CH_2)_2CHCH_3$	86.18	1, 149	0.6643^{20}	1.3765^{20}	−163	63	<−7	
m359	2-Methyl-1,5-pentanediamine	$H_2N(CH_2)_3CH(CH_3)CH_2NH_2$	116.21	4, 270	0.860	1.4590^{20}	80			
m360	2-Methyl-2,4-pentanediol	$(CH_3)_2C(OH)CH_2CH(OH)CH_3$	118.18	1, 486	0.9216_4^{20}	1.4270^{20}	−50	198	102	misc aq
m361	4-Methylpentanenitrile	$(CH_3)_2CHCH_2CH_2CN$	97.16	2, 329	0.8035_4^{20}	1.4061^{20}	−51.1	156.5	45	s alc; misc eth
m362	Methyl pentanoate	$CH_3(CH_2)_3CO_2CH_3$	116.16	2, 301	0.875	1.3962^{20}		128	22	sl s aq; misc alc, eth
m363	2-Methylpentanoic acid	$CH_3CH_2CH_2CH(CH_3)CO_2H$	116.16	2^2, 288	0.9242_{20}^{20}	1.4135^{20}	−85	196.4	107	1.3 aq
m364	2-Methyl-1-pentanol	$CH_3CH_2CH_2CH(CH_3)CH_2OH$	102.18	1, 409	0.8262^{20}	1.4180^{20}		148	54	s alc, eth
m365	3-Methyl-3-pentanol	$(CH_3CH_2)_2C(CH_3)OH$	102.18	1, 411	0.8281^{20}	1.4186^{20}	−23.6	123	46	misc alc, eth; sl s aq
m366	4-Methyl-2-pentanol	$(CH_3)_2CHCH_2CH(OH)CH_3$	102.18	1, 410	0.8080^{20}	1.4112^{20}	−90	132	41	1.6 aq
m367	4-Methyl-2-pentanone	$(CH_3)_2CHCH_2COCH_3$	100.16	1, 691	0.7978^{20}	1.3958^{20}	−84	116.5	18	1.7 aq; misc alc, bz, eth
m368	2-Methyl-2-pentenal	$CH_3CH_2CH{=}C(CH_3)CHO$	98.15	1^4, 3471	0.861	1.4503^{20}		138	31	s alc

m369	4-Methyl-2-pentenoic acid	$(CH_3)_2CHCH{=}CHCO_2H$	114.14	2^2, 406	0.9529	1.4489	35	115^{20mm}	46	i aq; v s alc
m370	4-Methyl-3-penten-2-one	$(CH_3)_2C{=}CHCOCH_3$	98.15	1, 736	0.8653^{20}	1.4440^{20}	−59	129.5	31	3.1 aq
m370a	4-Methyl-2-pentyl acetate	$(CH_3)_2CHCH_2CH(CH_3)O_2CCH_3$	144.21		0.8805^{25}	1.3980^{20}		147.5	45	
m371	1-Methylpentylamine	$CH_3(CH_2)_3CH(NH_2)CH_3$	101.19	4, 190	0.767_4^{20}		−19	116–118	13	s aq, alc, PE
m372	3-Methyl-1-pentyn-3-ol	$CH_3CH_2C(CH_3)(OH)C{\equiv}CH$	98.15	1^2, 506	0.8688_4^{20}	1.4318^{20}	−30.6	122	26	13 aq, misc bz, acet PE, EtOAc; s eth
m373	4-Methylphenetole	$CH_3C_6H_4OCH_2CH_3$	136.19	6, 393	0.945	1.5044^{20}		189–191	70	
m374	*N*-(4-Methylphenyl)-acetamide	$CH_3C_6H_4NHCOCH_3$	149.19	12, 920	1.212^{15}		150–153	307		s alc, EtOAc, HOAc
m375	Methyl phenylacetate	$C_6H_5CH_2CO_2CH_3$	150.18	9, 434	1.044	1.5075^{20}		218	90	i aq; misc alc, eth
m376	2-Methyl-1-phenyl-2-propanol	$CH_6H_5CH_2C(CH_3)_2OH$	150.22	6, 523	0.974	1.5140^{20}	25–26	96^{18mm}	81	
m377	1-Methyl-3-phenyl-propylamine	$C_6H_5CH_2CH_2CH(CH_3)NH_2$	149.24	12, 1165	0.922	1.5123^{20}		222	97	
m378	3-Methyl-1-phenyl-2-pyrazolin-5-one		174.20	24, 20			129–130	287^{265mm}		
m379	Methyl phenyl sulfide	$C_6H_5SCH_3$	124.21	6, 297	1.058	1.5882^{20}	−15	188	57	i aq; s alc

Methyl octyl ketone, d19
Methyl oleate, m347
o-Methylolphenol, h106
2-Methyloxacyclopropane, p232
Methyl oxirane, p232

Methyl palmitate, m269a
Methyl pentyl ketone, h14
Methylphenols, c303 thru c305
Methyl-*m*-phenylene diisocyanate, t171

Methyl phenyl ether, m55
Methyl phenyl ketone, a31
2-Methyl-2-phenylpropane, b523
Methyl γ-picolinate, m413



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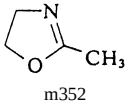

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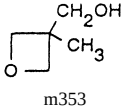

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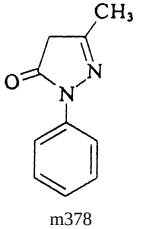

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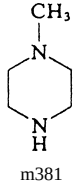
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
m380	*N*-Methyl-*N*-phenyl-urethane	$C_6H_5N(CH_3)CO_2CH_2CH_3$	179.22	12, 417	1.074	1.5149^{20}		243–244	>110	
m381	*N*-Methylpiperazine		100.17		0.903	1.4655^{20}		138	42	v s aq, alc, eth
m382	2-Methylpiperazine		100.17	23, 17			65–67	155.6	65	78 aq; 37 acet; 32 bz
m383	*N*-Methylpiperidine	$C_5H_{10}NCH_3$	99.19	20, 19	0.816	1.4378^{20}		106–107	3	v s aq; misc alc, eth
m384	2-Methylpiperidine	$CH_3C_5H_9N$	99.19	20, 95	0.844	1.4459^{20}	−5	119	8	v s aq; misc alc, eth
m385	3-Methylpiperidine	$CH_3C_5H_9N$	99.19	20, 100	0.845	1.4470^{20}		126	17	v s aq
m386	4-Methylpiperidine	$CH_3C_5H_9N$	99.19	20, 101	0.838	1.4458^{20}		124	7	v s aq
m387	1-Methyl-3-piperdine-methanol		129.20	21^2, 8	1.013	1.4772^{20}		140–145	94	
m388	1-Methyl-4-piperidone		113.16	21^2, 215	0.920	1.4614^{20}			60	
m389	2-Methylpropan-aldehyde	$(CH_3)_2CHCHO$	72.11	1, 671	0.7891^{20}	1.3727^{20}	−65	64.1	−40	9 aq; misc alc, bz, chl, eth
m390	2-Methylpropane	$(CH_3)_3CH$	58.12	1, 124		1.3810^{-25}	−138	−11.7	−87	13 mL aq; 1320 mL alc; 2890 mL eth
m391	*N*-Methyl-1,3-propane-diamine	$H_2NCH_2CH_2CH_2NHCH_3$	88.15	4^1, 419	0.844	1.4468^{20}		139–141	35	
m392	2-Methyl-1,2-propane-diamine	$(CH_3)_2C(NH_2)CH_2NH_2$	88.15	4, 266	0.841	1.4410^{20}			23	
m393	2-Methyl-1,3-propane-diol	$HOCH_2CH(CH_3)CH_2OH$	90.12	1, 480	1.015	1.4450^{20}	−91	125^{20mm}	>110	
m394	1-Methyl-1-propane-thiol	$CH_3CH_2CH(SH)CH_3$	90.19	1, 373	0.8246_4^{25}	1.4338^{25}	−165	84–85	21	sl s aq; v s alc, eth
m395	2-Methyl-1-propane-thiol	$(CH_3)_2CHCH_2SH$	90.19	1, 378	0.8357^{20}	1.4396^{20}	−79	88.5	−9	v s alc, eth
m396	2-Methyl-2-propane-thiol	$(CH_3)_3CSH$	90.19	1, 383	0.7943_4^{25}	1.4198^{25}	1.1	64.1	−4	i aq
m397	2-Methyl-1-propanol	$(CH_3)_2CHCH_2OH$	74.12	1, 373	0.8016^{20}	1.3958^{20}	−108	108	28	10 aq; misc alc, eth
m398	2-Methyl-2-propanol	$(CH_3)_3COH$	74.12	1, 379	0.7888^{20}	1.3877^{20}	25.8	82.4	11	misc aq, alc, eth
m399	2-Methylpropene	$(CH_3)_2C{=}CH_2$	56.11	1, 207	0.6266_4^{mp}		−140	−6.9		v s alc, eth
m400	2-Methyl-2-propen-1-ol	$H_2C{=}C(CH_3)CH_2OH$	72.11	1, 443	0.857	1.4260^{20}		113–115	33	
m401	Methyl propionate	$CH_3CH_2CO_2CH_3$	85.11	2, 239	0.915_4^{20}	1.3770^{20}	−88	79.7	6	6 aq; misc alc, eth

m402	Methyl propionyl-acetate	$C_2H_5COCH_2CO_2CH_3$	130.15	3[3], 1212	1.037	1.4220^{20}		74^{5mm}	71	
m403	4′-Methylpropio-phenone	$CH_3C_6H_4COCH_2CH_3$	148.21	7, 317	0.993	1.5280^{20}	7.2	238–239	96	
m404	Methyl propyl ether	$CH_3CH_2CH_2OCH_3$	74.12	1, 354	0.738^{20}			39.1		sl s aq; misc alc, eth
m405	2-Methyl-2-propyl-1,3-propanediol	$CH_3CH_2CH_2C(CH_3)(CH_2OH)_2$	132.20	1[1], 254		58–60	232	>110		
m406	Methyl propyl sulfide	$CH_3SCH_2CH_2CH_3$	90.18	1[3], 1432	0.8424^{20}	1.4442^{20}	−113.0	95.5		s aq
m407	Methyl 2-propynyl ether	$CH_3OCH_2C{\equiv}CH$	70.09	1, 4541	0.830	1.3961^{20}		62	−18	
m408	2-Methylpyrazine		94.12	23, 94	1.030	1.5042^{20}	−29	135	50	v s aq, alc, eth
m409	2-Methylpyridine	$CH_3C_5H_4N$	93.13	20, 234	0.9443^{20}	1.4957^{20}	−66.7	129	39	misc aq; s alc, eth
m410	3-Methylpyridine	$CH_3C_5H_4N$	93.13	20, 239	0.9566^{20}	1.5040^{20}	−18.3	144	36	misc aq, alc, eth
m411	4-Methylpyridine	$CH_3C_5H_4N$	93.13	20, 240	0.9548^{20}	1.5037^{20}	3.8	145	57	misc aq, alc, eth
m412	Methyl 3-pyridine-carboxylate	$(C_5H_4N)CO_2CH_3$	137.14	22, 39			39	209		s aq, alc, bz
m413	Methyl 4-pyridine-carboxylate	$(C_5H_4N)CO_2CH_3$	137.14	22, 46	1.001	1.5122^{20}	8.5	207–209	82	
m414	1-Methyl-2-pyridone		109.13	21, 268	1.112	1.5690^{20}	30–32	250^{740mm}	>110	

Methylpiperidinol, h152
Methyl pivalate, m235
2-Methyl-1-propanamine, i66
2-Methyl-2-propanamine, b511
1-Methyl-1-propanethiol, b471
Methyl propargyl ether, m407
2-Methyl-2-propenenitrile, m30a
Methyl propenoate, m126
2-Methylpropenoic acid, m29
2-Methylpropionaldehyde, i79
2-Methylpropionamide, i70
2-Methylpropionic acid, i81
2-Methylpropionic anhydride, i82
2-Methylpropionitrile, i83
1-Methylpropyl acetate, b502
2-Methylpropyl acetate, i63
2-Methyl-2-propylamine, b511
2-Methylpropylamine, i66
(1-Methylpropyl)benzene, b522
(2-Methylpropyl)benzene, i67
2-Methylpropyl formate, i69
Methyl propyl ketone, p42
2-Methylpropyl-2-methylpropanoate, i70
Methyl pyridyl ketones, a53, a54, a55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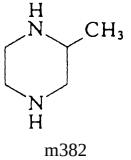
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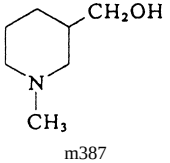
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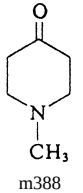
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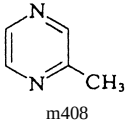
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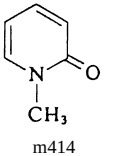
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TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

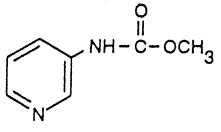
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
m415	Methyl 3-pyridyl-carbamate		152.15	22^{3}, 4076			121–123			
m416	2-[3-(6-Methyl-2-pyridyl)propoxy]-ethanol		195.26		1.052	1.5150^{20}			>110	
m417	*N*-Methylpyrrole		81.12	20, 163	0.914	1.4875^{20}	−57	112–113	15	i aq; misc alc, eth
m418	*N*-Methylpyrrolidine		85.15	20, 4	0.819_{4}^{20}	1.4247^{20}		80–81	−21	misc aq, eth
m419	*N*-Methyl-2-pyrrolidinone		99.13	21, 237	1.0279^{25}	1.4680^{25}	−24.4	202	96	misc aq, alc, bz, eth
m420	2-Methylquinoline		143.19	20, 387	1.058	1.6108^{20}	−2	248	79	i aq; s chl, eth
m421	4-Methylquinoline		143.19	20, 395	1.0826_{4}^{20}	1.6200^{20}	9–10	263	>110	misc alc, bz, eth
m422	6-Methylquinoline		143.19	20, 397	1.063	1.6140^{20}		259	>110	
m423	2-Methylquinozaline		144.18	23^{1}, 44	1.118	1.6156^{20}	180	245–247	107	misc aq
m424	Methyl salicylate	$HOC_6H_4CO_2CH_3$	152.15	10, 70	1.1831^{20}	1.5360^{20}	−8	223	96	0.7 aq; misc alc, HOAc; s chl, eth
m425	α-Methylstyrene	$C_6H_5C(CH_3)=CH_2$	118.18	5, 484	0.909	1.5375^{20}	−24	165.5	45	
m426	4-Methylstyrene	$CH_3C_6H_4CH=CH_2$	118.18	5, 485	0.897	1.5412^{20}		170–175	45	
m427	*mono*-Methyl succinate	$HO_2CCH_2CH_{162}CO_2CH_3$	132.12	2, 608			56–59	151^{20mm}		
m428	Methyl tetradecanoate	$CH_3(CH_2)_{12}CO_2CH_3$	242.40	2^{2}, 326	0.855	1.4362^{20}	18.4	323	>110	misc alc, bz, eth
m429	2-Methyltetrahydro-furan		86.13	17, 12	0.8552^{20}	1.4056^{20}		78	−11	
m430	3-Methyltetrahydro-pyran		100.16	17^{3}, 77	0.863	1.4204^{20}		109^{733mm}	6	
m431	3-Methyltetrahydro-thiophene-1,1-dioxide		134.20		1.191	1.4772^{20}		276	>110	
m432	4-Methylthiazole		99.16	27.16	1.090	1.5257^{20}		134	32	
m433	4-Methyl-5-thiazole-ethanol		143.21	27,3, 1754	1.196	1.5508^{20}		135^{7mm}	>110	
m434	2-Methyl-2-thiazoline		101.17	27, 13	1.067	1.5200^{20}	−101	145	37	
m435	(Methylthio)aceto-nitrile	CH_3SCH_2CN	87.14		1.039	1.4826^{20}		63^{15mm}	67	
m436	3-(Methylthio)aniline	$CH_3SC_6H_4NH_2$	139.22	13^{1}, 141	1.130	1.6423^{20}		165^{16mm}	>110	

m437	4-(Methylthio)benz-aldehyde	$CH_3SC_6H_4CHO$	152.22	8[1], 533	1.144	1.6452^{20}		90^{1mm}	>110	
m438	2-(Methylthio)benzo-thiazole		181.28	27, 109			43–46		>110	
m439	3-(Methylthio)-2-butanone	$CH_3CH(SCH_3)COCH_3$	118.20	1[4], 3993	0.975	1.4710^{20}		$50–54^{20mm}$	44	
m440	Methyl thiocyanate	CH_3SCN	73.12	3, 175	1.068^{20}	1.4680^{20}	−5	133	38	i aq; misc alc, eth
m441	2-Methylthiophene		98.17	17, 37	1.0193^{20}	1.5199^{20}	−63	113	7	
m442	3-Methylthiophene		98.17	17, 38	1.0218^{20}	1.5180^{20}	−69	115.4	11	i aq; misc alc, eth

1-Methyl-2-(3-pyridyl)pyrrolidine, n19
Methyl pyruvate, m355
Methyl stearate, m346

Methyl succinyl chloride, m195
Methylsulfonic acid, m34
Methyl theobromine, c1

Methyl thienyl ketone, a57
Methyl thioglycolate, m298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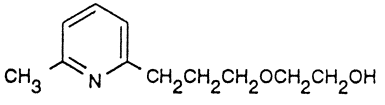
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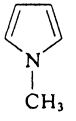
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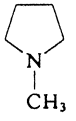
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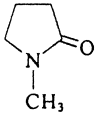
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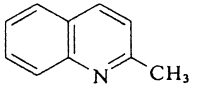
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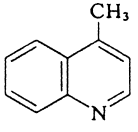
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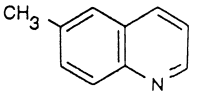
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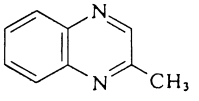
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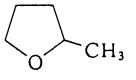
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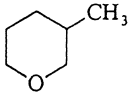
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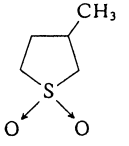
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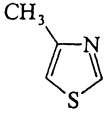
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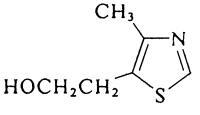
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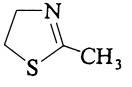
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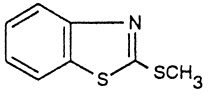
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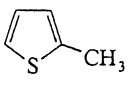
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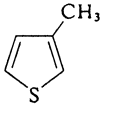
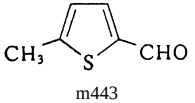

m442

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
m443	5-Methyl-2-thiophene-carboxaldehyde		126.18	17^{1}, 151	1.170	1.5860^{20}		114^{25mm}	82	
m444	*N*-Methyl-2-thiourea	$CH_3NHC(=S)NH_2$	90.15	4, 70			119–121			v s aq, alc
m445	*N*-Methyl-*o*-toluamide	$CH_3C_6H_4CONHCH_3$	149.19	9, 465	1.158^{15}		69–71			
m446	*N*-Methyl-*p*-toluene-sulfonamide	$CH_3C_6H_4SO_2NHCH_3$	185.25	11, 105			76–79			
m447	Methyl *p*-toluene-sulfonate	$CH_3C_6H_4SO_2OCH_3$	186.23	11, 99	1.234		27.5	145^{5mm}	>110	
m448	Methyltriacetoxysilane	$CH_3Si(O_2CCH_3)_3$	220.26	4^{3}, 1896	1.175_4^{20}	1.408^{20}	40–45	88^{3mm}	85	
m449	Methyl trichloro-acetate	$Cl_3CCO_2CH_3$	177.42	2, 208	1.488	1.4558^{20}		153	72	
m450	Methyltrichlorosilane	CH_3SiCl_3	149.48	4^{3}, 1896	1.273	1.4110^{20}		66	−15	
m451	Methyltriethoxysilane	$CH_3Si(OCH_3)_3$	178.30	4, 629	0.895	1.3840^{20}		141–143	23	
m452	Methyl trifluoro-acetate	$F_3CCO_2CH_3$	128.05	2^{3}, 427	1.273	1.2907^{20}		43	−7	
m453	Methyl trifluoro-methanesulfonate	$F_3CSO_2OCH_3$	164.10	3^{4}, 34	1.450	1.3244^{20}		94–99	38	
m454	Methyl 3,4,5-tri-hydroxybenzoate	$(HO)_3C_6H_2CO_2CH_3$	184.15	10, 483			201–203			
m455	Methyltrimethoxy-silane	$CH_3Si(OCH_3)_3$	136.22	4^{4}, 4203	0.955	1.3703^{20}		102	11	
m456	Methyl trimethyl-acetate	$(CH_3)_3CCO_2CH_3$	116.16	2, 320	0.873	1.3900^{20}		101	6	
m457	*N*-Methyl-*N*-(tri-methylsilyl)tri-fluoroacetamide	$F_3CC(=O)N(CH_3)Si(CH_3)_3$	199.25		1.075	1.3802^{20}		132	25	
m458	(Methyl)triphenyl-phosphonium bromide	$[CH_3P(C_6H_5)_3]^+ Br^-$	357.24	16, 760			230–234			
m459	2-Methylundecanal	$CH_3(CH_2)_8CH(CH_3)CHO$	184.32		0.830_4^{15}	1.4321^{20}		171	93	s alc, eth
m460	Methyl urea	$CH_3NHCONH_2$	74.08	4, 64	1.204		101–102			v s aq, alc; i eth
m461	*N*-Methyl–*N*-vinyl-acetamide	$CH_3CON(CH_3)CH=CH_2$	99.13	4^{3}, 442	0.959	1.4829^{20}		70^{25mm}	58	

m462	Methyl vinyl ether	$CH_3OCH{=}CH_2$	58.08	1^3, 1857	0.7511_4^{20}	1.3947	−123	5.5	−56	0.8 aq; v s alc
m463	Morpholine		87.12	27, 5	1.0005^{20}	1.4548^{20}	−4.9	128	375	misc aq, alc, bz, eth
m464	4-Morpholinepropio-nitrile		140.19	27^3, 337	1.037	1.4715^{20}	21	121^{2mm}		
m465	*N*-Morpholino-1-cyclo-hexene		167.25		0.995	1.5128^{20}		120^{10mm}	68	
m466	3-(*N*-Morpholino)-1,2-propanediol		161.20		1.157		37–38	191^{30mm}	>110	
m467	Myrcene	$(CH_3)_2C{=}CHCH_2CH_2$-$C(=CH_2)CH{=}CH_2$	136.24	1, 264	0.8013^{20}	1.4709^{20}		167	39	s alc, chl, eth, HOAc
n1	1-Naphthaldehyde	$C_{10}H_7CHO$	156.18	7, 400	1.150_4^{20}	1.6520^{20}	1–2	161^{15mm}	>110	s alc, eth
n2	Naphthalene	$C_{10}H_8$	128.17	5, 531	1.162_4^{20}	1.5821^{100}	80	217.7	79	0.3 aq; 7 alc; 33 bz; 50 chl
n3	1-Naphthalene-carboxylic acid	$C_{10}H_7CO_2H$	172.18	9, 647			160–162	300		sl s aq; v s hot alc, eth
n4	1,5-Naphthalene-diamine	$C_{10}H_6(NH_2)_2$	158.20	13, 203			185–187			s hot aq, hot alc
n5	1,8-Naphthalene-diamine	$C_{10}H_6(NH_2)_2$	158.20	13, 204	1.1265_4^{99}	1.6828^{99}	66.5	205^{12mm}		sl s aq; s alc, eth

4-Methyl-2-thiouracil, h125
Methyl *o*-toluate, m309
Methyl *m*-toluate, m311
Methyltrichlorosilane, t242
Methyl trimethylacetate, m235
β-Methylumbelliferone, h148
Methyl undecyl ketone, t263
Methyl urethane, m187
Methyl valerate, m362
4-Methylvaleronitrile, m361
Methyl veratrate, m231
Michler′s ketone, b178
Monoethyl adipate, e177
Monoglyme, d505
Monomethyl adipate, m277
Monomethyl glutarate, m276
Monomethyl succinate, m278
4-Morpholinocarboxyaldehyde, f39
1-Morpholinocyclopentene, c403
4-Morpholinoethanol, h127
MSTFA, m457
Myristic acid, t44
Myristolyl chloride, t46
Myristyl alcohol, t45
Myristyl bromide, b36
Naphthacene, b7
1-Naphthaleneacetamide, n13
1-Naphthaleneacetonitrile, n16
1,2-(1,8-Naphthalene)benzene, f1
Naphthalenediols, d439 thru d442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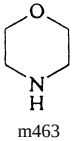
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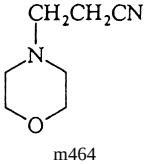
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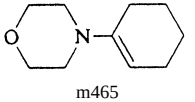
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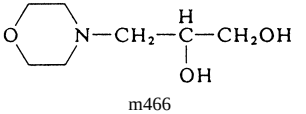
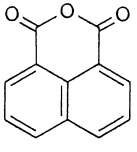

m466

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
n6	1-Naphthalenesulfonic acid	$C_{10}H_7SO_3H$	208.24	11, 155			90 dehydrates			v s aq, alc; sl s eth
n7	2-Naphthalenesulfonic acid	$C_{10}H_7SO_3H$	208.24	11, 171			124 dehydrates			v s aq, alc
n8	1,8-Naphthalic anhydride		198.18	17, 521			268			sl s HOAc
n9	1-Naphthol	$C_{10}H_7OH$	144.17	6, 596	1.0954_4^{99}	1.6206^{99}	96	288		v s alc, bz, chl, eth
n10	2-Naphthol	$C_{10}H_7OH$	144.17	6, 627	1.217^{4}		123	285	161	0.1 aq; 125 alc; 6 chl; 77 eth; s alk
n11	1,4-Naphthoquinone		158.16	7, 724	1.422		126			s bz, chl, eth, hot alc
n12	(2-Naphthoxy)acetic acid	$C_{10}H_7OCH_2CO_2H$	202.21	6, 645			155–157			
n13	2-(1-Naphthyl)-acetamide	$C_{10}H_7CH_2ONH_2$	185.23	9, 666			182			i aq; s bz, CS_2
n14	1-Naphthyl acetate	$C_{10}H_7O_2CCH_3$	186.21	6, 608			43–46		>110	s alc, eth
n15	1-Naphthylacetic acid	$C_{10}H_7CH_2CO_2H$	186.21	9, 666			135	dec		3.3 alc; v s chl, eth
n16	1-Naphthylacetonitrile	$C_{10}H_7CH_2CN$	167.21	9, 667		1.6192^{20}	33–35	194^{18mm}	>110	s alc
n17	1-Naphthylamine	$C_{10}H_7NH_2$	143.18	12, 1212	1.123_{25}^{25}	1.6703	50	301	157	0.2 aq; v s alc, eth
n18	1-Naphthyl isocyanate	$C_{10}H_7NCO$	169.19	12, 1244	1.177	1.6344^{20}	4	267	>110	
n19	Nicotine		162.24	23, 117	1.0097_4^{20}	1.5882^{20}	−79	123^{17mm}	101	misc aq; v s alc, eth, PE
n20	Nitrilotriacetic acid	$N(CH_2CO_2H)_3$	191.14	4, 369			242 dec			0.1 aq; s hot alc
n21	3′-Nitroacetophenone	$O_2NC_6H_4COCH_3$	165.15	7, 288			76–78	202		s alc, eth
n22	4′-Nitroacetophenone	$O_2NC_6H_4COCH_3$	165.15	7, 288			78–80	202		s alc
n23	2-Nitroaniline	$O_2NC_6H_4CH_2$	138.13	12, 687	1.442^{15}		71	284		s hot aq, alc, chl
n24	3-Nitroaniline	$O_2NC_6H_4CH_2$	138.13	12, 698	1.43		114	306		0.1 aq; 5 alc; 6 eth
n25	4-Nitroaniline	$O_2NC_6H_4CH_2$	138.13	12, 711	1.437^{14}		147	332	165	4 alc; 3.3 eth; s bz
n26	3-Nitrobenzaldehyde	$O_2NC_6H_4CHO$	151.12	7, 250	1.2792_4^{20}		58	164^{23mm}		s alc, chl, eth
n27	4-Nitrobenzaldehyde	$O_2NC_6H_4CHO$	151.12	7, 256	1.496		106–107			s alc, bz, HOAc
n28	2-Nitrobenzamide	$O_2NC_6H_4CONH_2$	166.12	9, 373	1.462^{32}		174–178	317		s hot aq, hot alc, eth
n29	3-Nitrobenzamide	$O_2NC_6H_4CONH_2$	166.12	9, 381			140–143			
n30	Nitrobenzene	$C_6H_5NO_2$	123.11	5, 233	1.205_4^{15}	1.5546^{15}	5.8	210.8	88	v s alc, bz, eth

n31	3-Nitrobenzene-1,2-dicarboxylic acid	$O_2NC_6H_3(CO_2H)_2$	211.13	9, 823			216 dec			2 aq; v s hot alc
n32	5-Nitrobenzene-1,3-dicarboxylic acid	$O_2NC_6H_3(CO_2H)_2$	211.13	9, 840			260			0.15 aq; v s alc, eth
n33	2-Nitrobenzenesulfonyl chloride	$O_2NC_6H_4SO_2Cl$	221.62	11, 67			65–67			s eth; d hot aq, alc
n34	5-Nitrobenzimidazole		163.14	23, 135			207–209			s alc, acid
n35	2-Nitrobenzoic acid	$O_2NC_6H_4CO_2H$	167.12	9, 370	1.58		146–148			0.7 aq; 33 alc; 22 eth
n36	3-Nitrobenzoic acid	$O_2NC_6H_4CO_2H$	167.12	9, 376	1.494		140–142			0.3 aq; 33 alc; 40 acet
n37	4-Nitrobenzoic acid	$O_2NC_6H_4CO_2H$	167.12	9, 389	1.58		242.8			9 alc; 2 eth; 5 acet
n38	4-Nitrobenzonitrile	$O_2NC_6H_4CN$	148.12	9, 397			146–149			s HOAC; sl s aq, alc
n39	3-Nitrobenzoyl chloride	$O_2NC_6H_4COCl$	185.57	9, 381			32–35	275–278	>110	dec aq, alc; v s eth
n40	4-Nitrobenzoyl chloride	$O_2NC_6H_4COCl$	185.57	9, 394			75	205^{105mm}		dec aq, alc; s eth
n41	2-Nitrobenzyl alcohol	$O_2NC_6H_4CH_2OH$	153.14	6, 447			70–72	270		
n42	3-Nitrobenzyl alcohol	$O_2NC_6H_4CH_2OH$	153.14	6, 449			30–32	180^{3mm}	>110	s aq, alc, eth
n43	4-Nitrobenzyl alcohol	$O_2NC_6H_4CH_2OH$	153.14	6, 450			92–94	185^{12mm}		v s alc, eth; sl s aq
n44	4-Nitrobenzyl bromide	$O_2NC_6H_4CH_2Br$	216.04	5, 334			98–100			2 alc; v s eth

1-Naphthol-2-carboxylic acid, h158
3-Naphthol-2-carboxylic acid, h160
1-Naphthonitrile, c327
1-Naphthylamine, a228
N-1-Naphthylaniline, p132
1-Naphthyl bromide, b376
1-Naphthyl chloride, c185
Natural orange 6, h161
NBA, b247
NBS, b422
Neohexane, d567
Neohexene, d574
Neopentane, d673
Neopentyl alcohol, d676
Neopentyl glycol, d594
Neophyl chloride, c178
Neral, d666
Nicotinaldehyde, p262
Nicotinic acid, p266
Nicotinonitrile, c329
Ninhydrin, i13
Nioxime, c361
2,2′,2″-Nitrilotriethanol, t266
1,1′,1″-Nitrilotris(2-propanol), t325
2-Nitro-*p*-anisidine, m89
5-Nitro-*o*-anisidine, m90
Nitroanisoles, m81, m92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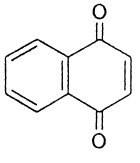
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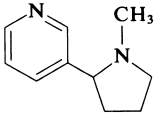
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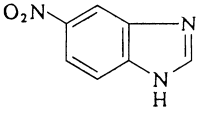

n34

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

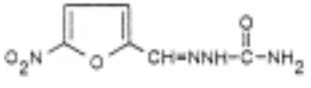
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
n45	4-Nitrobenzyl chloride	$O_2NC_6H_4CH_2Cl$	171.58	5, 329			70–73			8 alc; s eth
n46	2-Nitrobiphenyl	$O_2NC_6H_4C_6H_5$	199.21	5, 582	1.44_4^{25}	1.613^{25}	36.7	325	179	s alc, acet, CCl_4
n47	4-Nitrobiphenyl	$O_2NC_6H_4C_6H_5$	199.21	5, 583			112–114	340		sl s alc; s chl, eth
n48	1-Nitrobutane	$CH_3CH_2CH_2CH_2NO_2$	103.18	1, 123	0.975_{20}^{20}	1.4112	−81.3	152.8	47	sl s aq; misc alc, eth
n49	3-Nitro-2-butanol	$CH_3CH(NO_2)CH(OH)CH_3$	119.12	1, 373	1.1296_4^{25}	1.4414^{20}		92^{10mm}	91	
n50	3-Nitrocinnamic acid	$O_2NC_6H_4CH{=}CHCO_2H$	193.16	Merck: 12, 6692			200–201			1 alc
n51	2-Nitrodiphenylamine	$O_2NC_6H_4NHC_6H_5$	214.22	12, 690			76			i aq; s alc
n52	Nitroethane	$CH_3CH_2NO_2$	75.07	1, 99	1.0528_{20}^{20}	1.3920^{20}	−90	114	28	4.5 aq; misc alc, eth; s alk, chl
n53	5-Nitro-2-furaldehyde semicarbazone		198.14	17^3, 4467			242–244			s alk, chl, alk; 0.2 alc
n54	1-nitroguanidine	$O_2NNHC(=NH)NH_2$	104.07	3, 126			dec >225			0.4 aq; sl s MeOH
n55	5-Nitro-1*H*-indazole		163.14	23, 129			207–209			s alc, bz, eth, acet
n56	Nitromethane	CH_3NO_2	61.04	1, 74	1.1322_4^{25}	1.3795^{25}	−28.4	101.2	35	11 aq; s alc, eth
n57	1-Nitronaphthalene	$C_{10}H_7NO_2$	173.17	5, 553	1.223		59–60	304		s alc; v s chl, eth
n58	3-Nitro-2-pentanol	$CH_3CH_2CH(NO_2)CH(OH)CH_3$	133.15	1, 385	1.0818_4^{25}	1.4430^{20}		100^{10mm}	90	
n59	2-Nitrophenol	$O_2NC_6H_4OH$	139.11	6, 213	1.495		45	216		s alc, bz, eth, alk
n60	4-Nitrophenol	$O_2NC_6H_4OH$	139.11	6, 226	1.270_4^{120}		113–114	279		s aq; v s alc, chl, eth
n61	4-Nitrophenyl acetate	$O_2NC_6H_4O_2CCH_3$	181.15	6, 233			77–79			s aq; v s alc, bz, eth
n62	2-Nitrophenylacetic acid	$O_2NC_6H_4CH_2CO_2H$	181.15	9, 454			139–142			s hot aq, alc
n63	4-Nitrophenylacetic acid	$O_2NC_6H_4CH_2CO_2H$	181.15	9, 455			153–155			s alc, bz, eth; sl s aq
n64	4-Nitrophenylaceto-nitrile	$O_2NC_6H_4CH_2CN$	162.15	9, 456			115–117			s alc, eth; i aq
n65	2-Nitro-1,4-phenylene-diamine	$O_2NC_6H_3(NH_2)_2$	153.14	13, 120			137–140			
n66	4-Nitro-1,2-phenylene-diamine	$O_2NC_6H_3(NH_2)_2$	153.14	13, 29			199–201			sl s aq; s HCl
n67	4-Nitrophenyl-hydrazine	$O_2NC_6H_4NHNH_2$	153.14	15, 468			156 dec			s alc, chl, eth, hot bz

n68	2-Nitrophenyl phenyl ether	$O_2NC_6H_4OC_6H_5$	215.21	6[2], 222	1.2539^{20}	1.575^{20}	< −20	184^{8mm}		s alc, eth
n69	4-Nitrophenyl phenyl ether	$O_2NC_6H_4OC_6H_5$	215.21	6, 232			53–56	320	>110	s bz, eth
n70	3-Nitro-1,2-phthalic acid	$O_2NC_6H_3(CO_2H)_2$	211.13	9, 823			213–216 dec			
n71	4-Nitro-1,2-phthalic acid	$O_2NC_6H_3(CO_2H)_2$	211.13	9, 828			170–172			
n72	3-Nitrophthalic anhydride		193.11	17, 486			163–165			sl s aq, bz
n73	1-Nitropropane	$CH_3CH_2CH_2NO_2$	89.09	1, 115	1.0009^{20}	1.4016^{20}	−108	131.1	36	1.4 aq; misc org solv
n74	2-Nitropropane	$(CH_3)_2CHNO_2$	89.09	1, 116	0.9821^{20}	1.3949^{20}	−91.3	120.3	24	1.7 aq; misc org solv
n75	2-Nitro-1-propanol	$CH_3CH(NO_2)CH_2OH$	105.09	1, 358	1.1841^{25}_{4}	$1,4379^{20}$		99^{10mm}	100	s aq, alc, eth
n76	4-Nitropyridine-*N*-oxide	$O_2NC_5H_4N(\rightarrow O)$	140.10	20[3], 2528			159–162			
n77	Nitrosobenzene	C_6H_5NO	107.11	6, 230			67–69	59^{18mm}		
n78	*N*-Nitrosodimethylamine	$(CH_3)_2NNO$	74.08	8, 84	1.0048^{20}_{4}	1.4368^{20}		151	61	v s aq, alc, eth
n79	4-Nitrosodiphenylamine	$C_6H_5NC_6H_4NO$	198.22	Merck: 12, 6737			144–145			v s alc, bz, chl, eth
n80	1-Nitroso-2-naphthol	$C_{10}H_6(NO)OH$	173.16	7, 712			109–110			3 alc; s bz, eth, alk; 0.1 aq
n81	1-Nitroso-2-naphthol-3,6-disulfonic acid disodium salt hydrate		377.26	11[2], 190			>300			2.5 aq; sl s alc

4-Nitrobenzyl cyanide, n64
Nitrocresols, m339, m340

Nitroglycerine, g22
5-Nitroisophthalic acid, n32

3-Nitrophenyl disulfide, b216
3-Nitro-*o*-phthalic acid, n31



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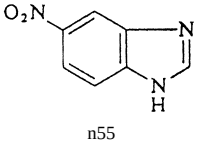

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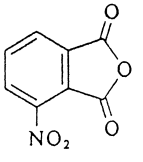

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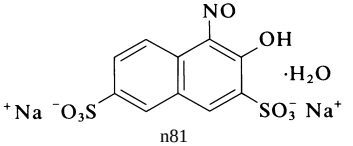


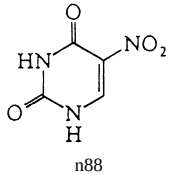
n81

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
n82	4-Nitrosophenol	HOC_6H_4NO	123.11	7, 622			126	dec 144		s aq; v s alc, eth; explodes on contact with conc acid, alk, or fire
n83	2-Nitrotoluene	$CH_3C_6H_4NO_2$	137.14	5, 318	1.1622^{19}_{15}	1.5472^{20}	−10	222	106	s alc, bz
n84	3-Nitrotoluene	$CH_3C_6H_4NO_2$	137.14	5, 321	1.1581^{20}_{4}	1.5459^{20}	15.5	231.9	101	misc alc, eth; s bz
n85	4-Nitrotoluene	$CH_3C_6H_4NO_2$	137.14	5, 323	1.392		52	238	106	s alc, bz, chl, eth
n86	2-Nitro-α,α,α-trifluorotoluene	$CF_3C_6H_4NO_2$	191.11	5[2], 251			31–32	105^{20mm}	95	v s alc, bz
n87	3-Nitro-α,α,α-trifluorotoluene	$CF_3C_6H_4NO_2$	191.11	5, 327	1.436^{16}_{4}	1.4715^{20}	−2.4	200–205	87	s alc, eth
n88	5-Nitrouracil		157.09	24, 320			>300			
n89	Nonadecane	$CH_3(CH_2)_{17}CH_3$	268.51	1, 174	0.7776^{32}_{4}	1.4335^{38}	32	330	168	s eth; sl s alc
n90	Nonane	$CH_3(CH_2)_7CH_3$	128.26	1, 165	0.7176^{20}_{4}	1.4054^{20}	−53.5	150.8	31	s abs alc, eth
n91	1,9-Nonanediamine	$H_2N(CH_2)_9NH_2$	158.29	4, 272			37–38	258	>110	
n92	Nonanedinitrile	$NC(CH_2)_7CN$	150.23	2, 709	0.929	1.4460^{20}		176^{11mm}	>110	v s alc, bz, eth
n93	1,9-Nonanedioic acid	$HO_2C(CH_2)_7CO_2H$	188.22	2, 707	1.029^{20}_{4}		106.5	286^{100mm}		0.24 aq; v s alc; 3 eth
n94	1,9-Nonanediol	$HO(CH_2)_7OH$	160.26	1, 493			47–49	177^{15mm}	>110	
n95	Nonanenitrile	$CH_3(CH_2)_7CN$	139.24	2, 354	0.851^{15}_{4}	1.4260^{20}	−34.2	224.0	81	s alc, eth
n96	Nonanoic acid	$CH_3(CH_2)_7CO_2H$	158.24	2, 352	0.906^{20}_{4}	1.4330^{20}	12.5	254.5	100	s alc, chl, eth
n97	γ-Nonanoic lactone		156.23	17, 245	0.976	1.4475^{20}		122^{6mm}	>110	
n98	1-Nonanol	$CH_3(CH_2)_8OH$	144.26	1, 423	0.8279^{20}_{4}	1.4338^{20}	−5.5	215	75	0.6 aq; misc alc, eth
n99	2-Nonanone	$CH_3(CH_2)_6COCH_3$	142.24	1, 709	0.832	1.4210^{20}	−21	192^{743mm}	64	
n100	3-Nonanone	$CH_3(CH_2)_5COCH_2CH_3$	142.24	1, 709	0.821	1.4204^{20}		187–188	67	
n101	5-Nonanone	$(CH_3CH_2CH_2CH_2)_2CO$	142.24	1, 710	0.806^{20}_{4}	1.4190^{20}	−50	186–187	60	misc alc, eth
n102	Nonanoyl chloride	$CH_3(CH_2)_7COCl$	176.69	2, 353	0.946^{15}_{4}	1.4377^{20}	−60.5	215.4	95	dec aq, alc; s eth
n103	3-Nonen-2-one	$CH_3(CH_2)_4CH{=}CHCOCH_3$	140.23	1[3], 3017	0.848	1.4484^{20}		85^{12mm}	81	
n104	Nonyl aldehyde	$CH_3(CH_2)_7CHO$	142.24	1, 708	0.827^{19}_{19}	1.4240^{20}		185	63	
n105	Nonylamine	$CH_3(CH_2)_8NH_2$	143.27	4, 198	0.782	1.4330^{20}		201	62	sl s aq; s alc, eth
n106	Nopol		166.26	6[3], 396	0.973	1.4930^{20}		230–240	98	
n107	Norbornane		96.17	5[1], 45			82–84			s alc
n108	2-Norbornanone		110.16	7, 57			94–96	168–172	33	

n109	*exo*-2-Norbornyl formate		140.18	6,3, 219	1.048	1.4622^{20}		67^{16mm}	53	
n110	(+)-Norephedrine	$C_6H_5CH(OH)CH(CH_3)NH_2$	151.21	13^2, 371			51–54		>110	
o1	*cis*,*cis*-9,12-Octadecadienoic acid	$CH_3(CH_2)_4CH{=}CHCH_2$-$CH{=}CH(CH_2)_7CO_2H$	280.44	2, 496	0.9025_4^{20}	1.4699^{20}	−5	230^{16mm}		v s eth; 10 PE; s abs alc
o2	Octadecanamide	$CH_3(CH_2)_{16}CONH_2$	283.50	2, 383			102–104	251^{12mm}		s hot alc, hot eth
o3	Octadecane	$CH_3(CH_2)_{16}CH_3$	254.50	1, 173	0.7767_4^{28}	1.4367^{28}	28.2	316.3	165	s acet, eth; sl s alc
o4	1-Octadecanethiol	$CH_3(CH_2)_{17}SH$	286.57	1,3, 1838		1.4648	31–35	360	185	s eth; sl s alc
o5	Octadecanoic acid	$CH_3(CH_2)_{16}CO_2H$	284.48	2, 377	0.847^{70}	1.4299^{80}	69	383		4.9 alc; 20 bz; 50 chl; 3.9 acet; 16.6 CCl_4; s toluene, pentyl acetate
o6	1-Octadecanol	$CH_3(CH_2)_{17}OH$	270.50	1, 431	0.8123_4^{58}	1.4388^{20}	59.6	203^{10mm}		s alc, eth
o7	9,12,15-Octadecatrienoic acid	$CH_3(CH_2CH{=}CH_2)_3CH_2$-$(CH_2)_6CO_2H$	278.44	2, 499	0.914_4^{18}	1.4800^{20}		230^{17mm}	>110	s alc, bz, eth
o8	1-Octadecene	$CH_3(CH_2)_{15}CH{=}CH_2$	252.49	1, 226	0.791_4^{18}	1.4439^{20}	17.7	314.9	148	s hot acet
o9	9-Octadecen-1-amine	$CH_3(CH_2)_7CH{=}CH(CH_2)_8NH_2$	267.50		0.813	1.4596^{20}			154	
o10	*cis*-9-Octadecenoic acid	$CH_3(CH_2)_7CH{=}CH(CH_2)_7CO_2H$	282.47	2, 463	0.8936_4^{20}	1.4581^{20}	13.4	360	189	s alc, bz, chl, eth

N-Nitrosophenylhydroxylamine, c317
Nitroso-R-salt, n81
3-Nitro-*o*-toluic acid, m334
3-Nitro-*p*-toluic acid, m336
4-Nitro-*m*-toluic acid, m331
6-Nitro-*m*-toluic acid, m337
2-Nitro-*p*-toluidine, m330
4-Nitro-*o*-toluidine, m328
5-Nitro-*o*-toluidine, m329
4-Nitroveratrole, d511
Nitroxylenes, d638 thru d641
Nonyl alcohol, n98
Nonyl iodide, i42
2,5-Norbornadiene, b134
exo-2-Norbornanamine, a245
5-Norbornen-2-carbaldehyde, b136
Norbornene, b135
Norbornylene, b135
Norcamphor, a104
Norleucine, a182
Norvaline, a248
NTA, n20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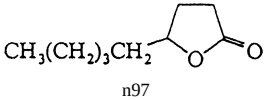
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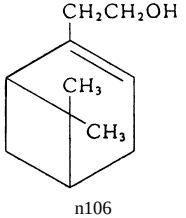
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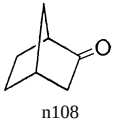
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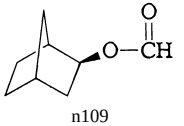
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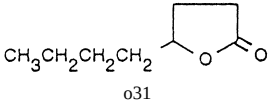
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
o11	*trans*-9-Octadecenoic acid	$CH_3(CH_2)_7CH{=}CH(CH_2)_7CO_2H$	282.47	2^{2}, 441	0.851^{79}	1.4308^{99}	44-45	288^{100mm}		s bz, chl, eth
o12	*cis*-9-Octadecen-1-ol	$CH_3(CH_2)_7CH{=}CH(CH_2)_8OH$	268.49	1, 453	0.850_4^{20}	1.4610^{20}	13–19	195^{8mm}	>110	s alc, eth; i aq
o13	9-Octadecenoyl chloride	$CH_3(CH_2)_7CH{=}CH{-}(CH_2)_7COCl$	300.92	2, 469	0.912	1.4630^{20}		180^{3mm}	>110	
o14	Octadecyl acrylate	$H_2C{=}CHCO_2(CH_2)_{17}CH_3$	324.55	2^{4}, 1468	0.800		32–34		>110	
o15	Octadecylamine	$CH_3(CH_2)_{17}NH_2$	269.52	4, 196	0.777^{27}		55–57	232^{32mm}	>110	s alc, bz, eth
o16	Octadecyl isocyanate	$CH_3(CH_2)_{17}NCO$	299.51	4^{3}, 439	0.847	1.4501^{20}	15–16	173^{5mm}	148	
o17	Octadecyltrichlorosilane	$CH_3(CH_2)_{17}SiCl_3$	387.94		0.984	1.4602^{20}		223^{10mm}	89	
o18	Octadecyl vinyl ether	$CH_3(CH_2)_{17}OCH{=}CH_2$	296.54		0.821_4^{30}	1.4440^{30}	28	187^{5mm}	177	
o19	1,7-Octadiene	$H_2C{=}CH(CH_2)_4CH{=}CH_2$	110.20		0.746	1.4220^{20}		114–121	9	
o20	1*H*,1*H*,5*H*-Octafluoro-1-pentanol	$HCF_2CF_2CF_2CF_2CH_2OH$	232.07	1^{4}, 1648	1.6647^{20}	1.3178^{20}		140–141	75	
o21	Octamethylcyclotetrasiloxane	$[\text{-}(CH_3)_2SiO\text{-}]_4$	296.62	4^{3}, 1885	0.956	1.3958^{20}	17–18	176	60	
o22	Octamethyltrisiloxane	$[(CH_3)_3SiO]_2Si(CH_3)_2$	236.54	4^{3}, 1879	0.8200^{20}	1.3848^{20}	*ca.* −80	153	29	s bz, PE; sl s alc
o23	Octane	$CH_3(CH_2)_6CH_3$	114.23	1, 159	0.7028_4^{20}	1.3974^{20}	−56.8	125.7	22	s eth; sl s alc
o24	1,8-Octanediamine	$H_2N(CH_2)_8NH_2$	144.26	4, 271			50–52	225–226	165	
o25	1,8-Octanedioic acid	$HO_2C(CH_2)_6CO_2H$	174.20	2, 691			140–144	230^{15mm}		0.16 aq; 0.6 eth; s alc
o26	1,2-Octanediol	$CH_3(CH_2)_5CH(OH)CH_2OH$	146.23	1^{3}, 2217			36–38	132^{10mm}	>110	
o27	1,8-Octanediol	$HO(CH_2)_8OH$	146.23	1, 490			59–61	172^{20mm}		v s alc; sl s aq, eth
o28	Octanenitrile	$CH_3(CH_2)_6CN$	125.22	2, 349	0.8135^{20}	1.4202^{20}	−45.6	198	73	s eth; sl s alc
o29	1-Octanethiol	$CH_3(CH_2)_7SH$	146.30	1^{3}, 1710	0.843	1.4525^{20}	−49.2	199.0	68	s alc
o30	Octanoic acid	$CH_3(CH_2)_6CO_2H$	144.21	2, 347	0.9088_4^{20}	1.4279^{20}	16.6	239	>110	0.07 aq; v s alc, chl, eth, PE
o31	γ-Octanoic lactone		142.20	17, 244	0.981	1.4440^{20}		234	>110	
o32	1-Octanol	$CH_3(CH_2)_7OH$	130.23	1, 418	0.8258_4^{20}	1.4290^{20}	−15.5	195	81	0.06 aq; misc alc, chl, eth
o33	(±)-2-Octanol	$CH_3(CH_2)_5CH(OH)CH_3$	130.23	1, 419	0.8193_4^{20}	1.4202^{20}	−31.6	175	71	0.1 aq; misc, alc, eth
o34	3-Octanol	$CH_3(CH_2)_4CH(OH)CH_2CH_3$	130.23	1^{1}, 208	0.819	1.4260^{20}		174–176	65	
o35	4-Octanol	$CH_3(CH_2)_3CH(OH)CH_2CH_2CH_3$	130.23		0.8192^{20}	1.425^{20}		176.6	71	
o36	2-Octanone	$CH_3(CH_2)_5COCH_3$	128.22	1, 704	0.819_4^{20}	1.4150^{20}	−16	173	52	i aq; misc alc, eth

o37	3-Octanone	$CH_3(CH_2)_4COCH_2CH_3$	128.22	1, 706	0.8220_4^{20}	1.4150^{20}		167–168	46	i aq; misc alc, eth
o38	4-Octanone	$CH_3(CH_2)_3COCH_2CH_2CH_3$	128.22	1, 706	0.809	1.4139^{20}		164	45	
o39	Octanoyl chloride	$CH_3(CH_2)_6COCl$	162.66	2, 348	0.955	1.4350^{20}	< -70	195	80	dec aq, alc; s eth
o40	1-Octene	$CH_3(CH_2)_5CH{=}CH_2$	112.22	1, 221	0.7149_4^{20}	1.4087^{20}	-102	121	21	i aq; misc alc, eth
o41	2-Octen-1-ylsuccinic anhydride		210.27		1.000	1.4694^{20}	8–12	168^{10mm}	>110	
o42	Octyl acetate	$CH_3CO_2(CH_2)_7CH_3$	172.27	2, 134	0.868	1.4185^{20}		211	88	sl s aq; misc alc
o43	Octyl aldehyde	$CH_3(CH_2)_6CHO$	128.22	1, 704	0.821_4^{20}	1.4183^{20}	12–15	171	51	sl s aq; misc alc
o44	Octylamine	$CH_3(CH_2)_7NH_2$	129.25	4, 196	0.782	1.4290^{20}	$-5/-1$	175–177	62	i aq; s alc, eth
o45	Octyl cyanoacetate	$NCCH_2CO_2(CH_2)_7CH_3$	197.28		0.934	1.4490^{20}		$95^{0.11mm}$	>110	
o46	Octyl gallate	$3,4,5\text{-}(HO)_3C_6H_2CO_2(CH_2)_7CH_3$	282.34	10^3, 2079			101–104			
o47	1-Octyl-2-pyrrolidine		197.32		0.920	1.4650^{20}	-25	172^{15mm}	>110	
o48	Octyltrichlorosilane	$CH_3(CH_2)_7SiCl_3$	247.67	4^3, 1907	1.070^{20}	1.4473^{20}		226^{730mm}	96	
o49	1-Octyne	$CH_3(CH_2)_5C{\equiv}CH$	110.19	1, 258	0.7457^{20}	1.4159^{20}	-79.3	126.2	17	i aq; s alc, eth
o50	1-Octyn-3-ol	$CH_3(CH_2)_4CH(OH)C{\equiv}CH$	126.20	1^3, 1996	0.864	1.4410^{20}		83^{19mm}	63	
o51	L-(+)-Ornithine	$H_2N(CH_2)_3CH(NH_2)CO_2H$	132.16	4, 420			140			v s aq, alc; sl s eth
o52	Oxalic acid	HO_2CCO_2H	90.04	2, 502	1.90_4^{17}		190 dec			14 aq^{20}; 40 alc; 1.3 eth
o53	Oxalic acid dihydrate	$HO_2CCO_2H \cdot 2H_2O$	126.07	2, 502	1.653_4^{19}		$-2H_2O$, 102			14 aq; 40 alc; 1 eth
o54	Oxalyl bromide	BrC(=O)C(=O)Br	215.84	2^1, 236		1.5220^{20}	-19	103^{720mm}	none	
o55	Oxalyl chloride	ClC(=O)C(=O)Cl	126.93	2, 542	1.455	1.4290^{20}	-10	64	none	s eth; viol dec aq, alc

Octadecyl bromide, b384
Octadecyl iodide, i43
Octadecyl mercaptan, o4
2,3,4,6,7,8,9,10-Octahydropyrimidol[1,2-*a*]azepine, d62
Octaldehyde, o43
Octamethylene glycol, o27
Octanal, o43
1,8-Octanedicarboxylic acid, d10
tert-Octylamine, t103
Octyl bromide, b385
Octyl chloride, c204
Octyl cyanide, n95
Octyldimethylamine, d649
Octyl ether, d729
Octyl iodide, i44
Octyl sulfide, d730
Oleic acid, o11
Oleoxyl chloride, o13
Oleyl alcohol, o12
Oleylamine, o9
o-Orthanilic acid, a115
7-Oxabicyclo[2.2.1]heptane, c331b, e7
7-Oxabicyclo[4.1.0]heptane, e6
6-Oxabicyclo[3.1.0]hexane, e10
Oxacyclopentane, t69



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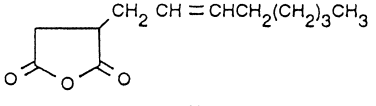

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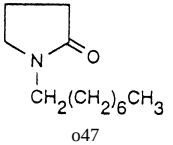

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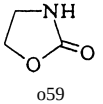
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
o56	Oxalyl dihydrazide	$H_2NNHC(=O)C(=O)NHNH_2$	118.10	2, 559			240 dec			s hot aq; sl s alc, eth
o57	Oxamic hydrazide	$H_2NC(=O)C(=O)NHNH_2$	103.08	2, 559			218 dec			s alk; sl s aq; i eth
o58	Oxamide	$H_2NC(=O)C(=O)NH_2$	88.07	2, 545	1.667_4^{20}		dec 350			sl s hot aq, alc
o59	2-Oxazolidone		87.08	27, 135			86–89	220^{48mm}		
o60	2-Oxobutyric acid	$CH_3CH_2C(=O)CO_2H$	102.09	3, 629	1.200_4^{17}	1.3972^{20}	32–34	82^{16mm}	81	v s aq, alc; v sl s eth
o61	2-Oxohexamethylene-imine		113.16	21^2, 216	1.02_4^{75}		69.2	270	125	84 aq; v s alc, eth, chlorinated HC's
o62	5-Oxohexanonitrile	$CH_3CO(CH_2)_3CN$	111.14	3^3, 1234	0.975	1.4328^{20}		240	107	
o63	4-Oxopentanoic acid	$CH_3COCH_2CH_2CO_2H$	116.12	3, 671	1.1447_4^{25}	1.4396^{20}	33–35	246	137	v s aq, alc, bz, eth
o64	2-Oxopropionaldehyde	$CH_3C(=O)CHO$	72.06	1, 762	1.0455^{24}	1.4209^{20}		72	none	s aq, alc
o65	2-Oxopropionic acid	$CH_3C(=O)CO_2H$	88.06	3, 608	1.267_4^{15}	1.4315^{20}	11.8	165 dec	82	misc aq, alc, eth
o66	2-Oxo-1-pyrrolidine-propionitrile		138.17		1.120	1.4880^{20}		$140^{0.3mm}$	>110	
o66a	2,2′-Oxybis[2-methyl]-propane	$(CH_3)_3COC(CH_3)_3$	130.23		0.7658	1.3949^{20}		107		dec acids
o67	2,2′-Oxydiacetic acid	$HO_2CCH_2OCH_2CO_2H$	134.09	3, 234			142–145	dec		v s aq, alc; sl s eth
o68	4,4′-Oxydianiline	$H_2NC_6H_4OC_6H_4NH_2$	200.24	13, 441			190–192		218	
o69	3,3′-Oxydipropio-nitrile	$NCCH_2CH_2OCH_2CH_2CN$	124.14		1.043	1.4405^{20}		$112^{0.5mm}$	>110	
p1	Paraformaldehyde	$(CH_2O)_x$		1, 566			165 dec		71	s(slow) aq; s alk; i alc, eth
p2	Paraldehyde	$[-HC(CH_3)O-]_3$	132.16	19, 385	0.9984^{15}	1.4049^{20}	12.6	124		11 aq; misc alc, chl
p3	Parathion	$(C_2H_5O)_2P(=S)C_6H_4NO_2$	291.27		1.26_4^{25}	1.5370^{25}	6	375		v s alc, bz, eth
p4	Pentabromophenol	C_6Br_5OH	488.62	6, 206			223–226			sl s alc, eth
p5	Pentachloroacetone	$Cl_2CHC(=O)CCl_3$	230.31	1, 690	1, 656	1.4967^{20}	21 (anhyd)	192	none	i aq; v s acet
p6	Pentachlorobenzene	C_6HCl_5	250.34	5, 205	1.8342^{16}		82–85	275–277	none	v s bz, chl, eth
p7	Pentachloroethane	Cl_2CHCCl_3	202.30	1, 87	1.6712_4^{25}	1.5030^{20}	−29.0	160	none	0.05 aq; misc alc, eth
p8	Pentachloronitro-benzene	$C_6Cl_5(NO_2)$	295.34	5, 247	1.718_4^{25}		140–143			s bz, chl
p9	Pentachlorophenol	C_6Cl_5OH	266.34	6, 194	1.978_4^{22}		190–191	310		v s alc; s bz; 148 eth
p10	Pentachloropyridine	C_5Cl_5N	251.33	20, 232			124–126			
p11	Pentadecane	$CH_3(CH_2)_{13}CH_3$	212.42	1, 172	0.7684_4^{20}	1.4319^{20}	9.9	270	132	v s alc, eth
p12	Pentadecanenitrile	$CH_3(CH_2)_{13}CN$	223.40	2^1, 163	0.825	1.4420^{20}	20–23	322	>110	
p13	8-Pentadecanone	$[CH_3(CH_2)_7]_2C=O$	226.40	1, 717			41–43	178	>110	s alc

p14	3-Pentadecylphenol	$CH_3(CH_2)_{14}C_6H_4OH$	304.52				50–53	195^{1mm}	>110	
p15	1,2-Pentadiene	$CH_3CH_2CH{=}C{=}CH_2$	68.12	1, 251	0.6926_4^{20}	1.4209^{20}	−137.3	44.9		
p16	*cis*-1,3-Pentadiene	$CH_3CH{=}CHCH{=}CH_2$	68.12	1, 251	0.6910^{10}	1.4363^{20}	−140.8	44.1	−28	
p17	*trans*-1,3-Pentadiene	$CH_3CH{=}CHCH{=}CH_2$	68.12	1, 251	0.6760^{20}	1.4301^{20}	−87.5	42.0	−28	
p18	1,4-Pentadiene	$H_2C{=}CHCH_2CH{=}CH_2$	68.12	1, 251	0.6608_4^{22}	1.3888^{20}	−148.3	26.0	4	
p19	Pentaerythritol	$C(CH_2OH)_4$	136.15	1, 528	1.38_4^{25}	1.548	260			6 aq; v sl s alc; i eth
p20	Pentaerythritol diacrylate monostrearate	$CH_3(CH_2)_{16}CO_2CH_2$-$C(CH_2O_2CCH{=}CH_2)_2$-CH_2OH	510.72		1.018		29–31		>110	
p21	Pentaerythritol triacrylate	$(H_2C{=}CHCO_2CH_2)_3CCH_2OH$	298.30		1.180	1.4864^{20}			>110	
p22	Pentaerythrityl tetranitrate	$C(CH_2ONO_2)_4$	316.15	1[2], 602	1.1773_4^{20}		140	explodes on shock		s acet; sl s eth, alc
p23	Pentaethylenehexamine	$H_2N(CH_2CH_2NH)_4CH_2CH_2NH_2$	232.38	4[4], 1245	0.950	1.5096^{20}			>110	
p24	Pentamethylbenzene	$C_6H(CH_3)_5$	148.25	5, 443	0.917_4^{20}	1.527^{20}	54.4	231	91	v s alc, bz
p25	1,2,3,4,5-Pentamethylcyclopentadiene		136.24		0.870	1.4733^{20}		58^{13mm}	44	

Oxapentadiene, f45
Oxetanone, p210
Oxirane, e147
2-Oxo-10-bornanesulfonic acid, c5
3-Oxobutanoic acid, a25
Oxolan-2-one, b617
3-Oxo-*N*-phenylbutanamide, a24
2,2′-Oxybis(chloroethane), b163
1,1′-Oxybis(chloromethane), b165a
1,1′-Oxybis(2-ethoxyethane), b186
1,1′-Oxybis(2-methoxyethane), b214
1,1′-Oxybis(3-methylbutane), d466a
1,1′-Oxybis(2-methylpropane), d458
1,1′-Oxybis(pentane), d738
2,2′-Oxybis(propane), d476
3,3′-Oxybis(1-propene), d31
2,2′-Oxydiethanethiol, b208
2,2′-Oxydiethanol, b198
Palmitic acid, h34
Pelargonaldehyde, n104
Pelargonic acid, n96
Pelargononitrile, n95
Pelargonoyl chloride, n102
Pentaerythritol diformal, t125
Pentalin, p7
Pentamethylene glycol, p32
Pentamethylene oxide, t83



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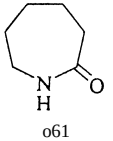

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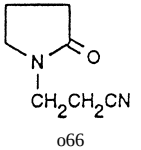

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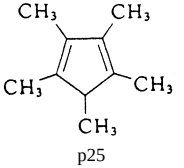

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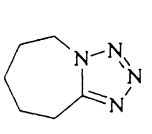
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
p26	*N,N,N′,N′,N″*-Pentamethyldiethylenetriamine	$[(CH_3)_2NCH_2CH_2]_2NCH_3$	173.30	4,*4*, 1245	0.830	1.4420^{20}	−20	198	53	
p27	1,5-Pentamethylenetetrazole		138.17	26^2, 213			59–61	194^{12mm}		
p28	Pentanal	$CH_3CH_2CH_2CH_2CHO$	86.13	1, 676	0.8095_4^{20}	1.3942^{20}	−92	103	12	1.4 aq; misc alc, eth
p29	Pentane	$CH_3CH_2CH_2CH_2CH_3$	72.15	1, 130	0.6262_4^{20}	1.3575^{20}	−129.7	36.0	−49	misc alc, eth
p30	1,5-Pentanediamine	$H_2N(CH_2)_5NH_2$	102.18	4, 266	0.873_4^{25}	1.4591^{20}	−129.7	178–180	62	s aq, alc; sl s eth
p31	1,2-Pentanediol	$CH_3CH_2CH_2CH(OH)CH_2OH$	104.15	1^2, 548	0.971	1.4397^{20}		206	104	
p32	1,5-Pentanediol	$HO(CH_2)_5OH$	104.15	1, 481	0.9941^{20}	1.4494^{20}	−18	239	129	s aq, alc; sl s eth
p33	2,3-Pentanedione	$CH_3CH_2C(=O)C(=O)CH_3$	100.11	1, 776	0.957	1.4068^{20}	−52	110–112	19	
p34	2,4-Pentanedione	$CH_3COCH_2COCH_3$	100.11	1, 777	0.9721^{25}	1.4510^{20}	−23.1	138	34	17 aq; misc alc, eth
p35	Pentanenitrile	$CH_3CH_2CH_2CH_2CN$	83.13	2, 301	0.8035_4^{15}	1.3991^{15}	−92	141.3	40	i aq; s alc, eth
p36	1-Pentanesulfonic acid, sodium salt	$CH_3(CH_2)_4SO_3^-\ Na^+$	174.19	4^3, 23			>300			4 aq
p37	1-Pentanethiol	$CH_3(CH_2)_4SH$	104.22	1, 384	0.840	1.4460^{20}	−75.7	126.6	18	i aq; misc alc, eth
p38	Pentanoic acid	$CH_3(CH_2)_3CO_2H$	102.13	2, 299	0.9390_4^{20}	1.4080^{20}	−33.7	186	96	2.4 aq; v s alc, eth
p39	1-Pentanol	$CH_3(CH_2)_4OH$	88.15	1, 383	0.8146_4^{20}	1.4100^{20}	−79	137.5	33	$2.7\ aq^{22}$; misc alc, eth
p40	2-Pentanol	$CH_3CH_2CH_2CH(OH)CH_3$	88.15	1, 384	0.8098_4^{20}	1.4054^{20}	−73	119.3	34	$16.6\ aq^{20}$; misc alc, eth
p41	3-Pentanol	$CH_3CH_2CH(OH)CH_2CH_3$	88.15	1, 385	0.8150_4^{25}	1.4077^{25}	−69	116	41	$5.5\ aq^{20}$; s alc, eth
p42	2-Pentanone	$CH_3CH_2CH_2COCH_3$	86.13	1, 676	0.8095^{20}	1.3900^{20}	−76.8	102	7	misc acet, bz, eth, PE
p43	3-Pentanone	$CH_3CH_2COCH_2CH_3$	86.13	1, 679	0.8143^{20}	1.3920^{20}	−39.0	102.0	13	3.4 aq
p44	Pentanophenone	$C_6H_5CO(CH_2)_3CH_3$	162.23	7, 327	0.988	1.5143^{20}		107^{5mm}	102	s alc, eth
p45	Pentanoyl chloride	$CH_3(CH_2)_3COCl$	120.58	2, 301	1.016	1.4216^{20}		125–127	32	
p46	1,4,7,10,13-Pentaoxacyclopentadecane	$[-CH_2CH_2O-]_5$	220.27		1.109	1.4650^{20}		$135^{0.2mm}$	>110	
p47	2,5,8,11,14-Pentaoxapentadecane	$CH_3(OCH_2CH_3)_4OCH_3$	222.28	1^3, 2107	1.0087_4^{20}	1.4330^{20}	−27	275–276	140	s aq; misc hydrocarbon solvents
p48	1-Pentene	$CH_3CH_2CH_2CH=CH_2$	70.14	1, 210	0.6429_4^{20}	1.3714^{20}	−165	30.1	−18	misc alc, bz, eth
p49	*cis*-2-Pentene	$CH_3CH_2CH=CHCH_3$	70.14	1, 210	0.6503_4^{20}	1.3813^{20}	−151	37.0	−20	misc alc, eth
p50	*trans*-2-Pentene	$CH_3CH_2CH=CHCH_3$	70.14	1, 210	0.6482_4^{20}	1.3792^{20}	−140	36.3	−45	misc alc, eth
p51	*cis*-2-Pentenenitrile	$CH_3CH_2CH=CHCN$	81.12	2^2, 400	0.820	1.4269^{20}		128	23	
p52	*trans*-3-Pentenenitrile	$CH_3CH=CHCH_2CN$	81.12	2, 427	0.837	1.4221^{20}		144–147	40	

p53	Pentyl acetate	$CH_3(CH_2)_4O_2CCH_3$	130.19	2, 131	0.8753^{20}	1.4020^{20}	−70.8	149.2	16	0.17 aq; misc alc, eth
p54	Pentylamine	$CH_3(CH_2)_4NH_2$	87.16	4, 175	0.7544^{20}	1.448^{20}	−55	104	−1	v s aq; misc eth; s alc
p55	Pentylbenzene	$CH_3(CH_2)_4C_6H_5$	148.25	5, 434	0.8594_4^{20}	1.4885^{20}	−78.3	202.2	65	s alc, misc bz, eth
p56	2-Pentylcinnam-aldehyde	$C_6H_5CH{=}C[(CH_2)_4CH_3]CHO$	202.30	7[2], 310	0.970	1.5571^{20}		290	>110	
p57	4-*tert*-Pentylphenol	$CH_3CH_2C(CH_3)_2C_6H_4OH$	164.25	6, 548	0.962_4^{20}		93	262		s alc, eth
p58	1-Pentyne	$CH_3CH_2CH_2C{\equiv}CH$	68.11	1, 250	0.6901_4^{20}	1.3852^{20}	−106	40.2	−34	v s alc; misc eth
p59	Perfluoro-1-octane-sulfonyl fluoride	$CF_3(CF_2)_7SO_2F$	502.12	2[4], 996	1.824	1.3010^{20}		154–155	none	
p60	Peroxyacetic acid	$CH_3C(=O)CO_2H$	76.05	2, 169	1.226_4^{15}	1.3876^{20}	−0.2	110	41	v s aq, alc, eth
p61	Petroleum ether	Principally pentanes and hexanes		Merck: 12, 7329	0.640	1.3630^{20}		35–60	−49	misc bz, chl, eth, CCl_4; s glacial HOAc
p62	Phenanthrene		178.23	5, 667	1.063		100	340		1.6 alc; 50 bz; 30 eth
p63	1,10-Phenanthroline		180.21	23, 227			114–117			0.3 aq; 1.4 bz; s alc, acet
p64	Phenethylisobutyrate	$(CH_3)_2CHCO_2CH_2CH_2C_6H_5$	192.26	6[2], 451	0.988	1.4880^{20}		250	108	

Pentamethylethyl alcohol, t362
1,5-Pentanedicarboxylic acid, h7
Pentanedinitrile, g17
Pentanedioic acid, g14
3,6,9,12,15-Pentaoxaheptadecane, t53
2,5,8,11,14-Pentaoxapentadecane, b212
Pentetic acid, d363
Pentyl alcohol, p39
sec-Pentyl alcohol, p40
tert-Pentyl alcohol, m162
sec-Pentylamine, a246
tert-Pentylamine, d682
Pentyl bromide, b387
Pentyl chloride, c204a
Pentyl cyanide, h61
Pentyl mercaptan, p37
Peracetic acid, p60
Perdeuterocyclohexane, c348
Perfluoropropane, h44
Perylene, d65
Phenacetin, e51
Phenacyl bromide, b251
Phenacyl chloride, c31
Phenazone, a299
1,2,4-Phenenyl triacetate, t193
Phenethyl acetate, p111
Phenethyl alcohol, p110
sec-Phenethyl alcohol, m149
Phenethylamine, p112
Phenethyl bromide, b334
Phenethyl chloride, c128
Phenetole, e36



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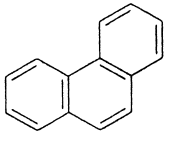
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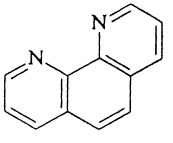

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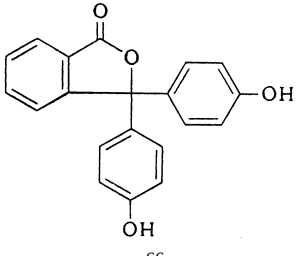
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
p65	Phenol	C_6H_5OH	94.11	6, 110	1.0576_4^{41}	1.5418^{41}	41	182	79	6.7 aq; 8.2 bz; v s alc, chl, eth, alk
p66	Phenolphthalein		318.33	18, 143	1.299		261–263			8.2 alc; 1 eth
p67	Phenothiazine		199.28	27, 63			185.1	371		v s bz; s eth; sl s alc
p68	Phenoxyacetic acid	$C_6H_5OCH_2CO_2H$	152.15	6, 161			98–100	285 sl dec		1.3 aq; v s alc, bz, HOAc, CS_2, eth
p69	Phenoxyacetyl chloride	$C_6H_5OCH_2COCl$	170.60	6, 162	1.235	1.5340^{20}		225–226	108	dec aq, alc; s eth
p70	4-Phenoxyaniline	$C_6H_5OC_6H_4NH_2$	185.23	13, 438			84	189^{14mm}		s hot aq; v s alc, eth
p71	2-Phenoxybutyric acid	$CH_3CH_2CH(OC_6H_5)CO_2H$	180.20	6, 163			79–83	258		sl s aq
p72	2-Phenoxyethanol	$C_6H_5OCH_2CH_2OH$	138.17	6, 146	1.102_4^{22}	1.5370^{20}	14	245.2	>110	s aq; v s alc, eth
p73	1-Phenoxy-2-propanol	$C_6H_5OCH_2CH(OH)CH_3$	152.19	6^1, 85	1.063_4^{25}	1.523^{20}	13–18	240	135	
p74	2-Phenoxypropionic acid	$CH_3CH(OC_6H_5)CO_2H$	166.18	6, 163			116–119	265		s alc; sl s aq
p75	3-Phenoxypropyl bromide	$C_6H_5O(CH_2)_3Br$	215.10	6, 142	1.365	1.5460^{20}		134^{14mm}	96	
p76	3-Phenoxytoluene	$C_6H_5OC_6H_4CH_3$	184.24	6, 377	1.051	1.5727^{20}		271–273	>110	
p77	Phenylacetaldehyde	$C_6H_5CH_2CHO$	120.15	7, 292	1.027_{25}^{25}	1.5290^{20}	33–34	195	86	sl s aq; s alc, eth
p78	Phenylacetaldehyde dimethyl acetal	$C_6H_5CH_2CH(OCH_3)_2$	166.22	7, 293	1.004	1.4930^{20}		221	83	
p79	Phenylacetaldehyde ethylene acetal		164.21	19^4, 220	1.100	1.5220^{20}		120^{12mm}	107	
p80	Phenyl acetate	$C_6H_5O_2CCH_3$	136.15	6, 152	1.073	1.5030^{20}		196	76	misc alc, eth, chl
p81	Phenylacetic acid	$C_6H_5CH_2CO_2H$	136.15	9, 431	1.091_4^{77}		76.5	265.5		s hot aq, alc, eth
p82	Phenylacetonitrile	$C_6H_5CH_2CN$	117.15	9, 441	1.0214	1.5233^{20}	−23.8	233.5	101	i aq; misc alc, eth
p83	Phenylacetyl chloride	$C_6H_5CH_2COCl$	154.60	9, 436	1.169	1.5325^{20}		95^{12mm}	102	dec aq, alc
p84	Phenylacetylene	$C_6H_5C{\equiv}CH$	102.14	5, 511	0.9300	1.5470^{20}	−44.9	142.4	31	misc alc, eth
p85	Phenylacetylurea	$C_6H_5CH_2CONHCONH_2$	178.19	Merck: 12, 7343			212–216			sl s alc, bz, chl, eth
p86	(±)-3-Phenylalanine	$C_6H_5CH_2CH(NH_2)CO_2H$	165.19	14, 495			271–273			1.4 aq
p87	Phenyl 4-amino-salicylate	$H_2NC_6H_3$-2-$(OH)CO_2C_6H_5$	229.24	Merck; 12, 7426			153			0.7 mg aq
p88	4-Phenylazoaniline	$C_6H_5N{=}NC_6H_4NH_2$	197.24	16^1, 310			123–126	>360		v s alc, bz, chl, eth

p89	Phenylazoformic acid 2-phenylhydrazide	$C_6H_5N{=}NCONHNHC_6H_5$	240.27	16, 24			156–159 dec			
p90	4-Phenylazophenol	$C_6H_5N{=}NC_6H_4OH$	198.23	16, 96			150–152	230^{20mm}		v s alc, eth
p91	2-Phenylbenzimidazole		194.24	23, 230			293–296			s abs alc; sl s bz, chl
p92	Phenyl benzoate	$C_6H_5CO_2C_6H_5$	198.22	9, 116	1.235		69–72	298–299		v s hot alc; sl s eth
p93	*N*-Phenylbenzylamine	$C_6H_5CH_2NHC_6H_5$	183.25	12, 1023	1.061		35–38	306–307	>110	s alc, chl, eth
p94	*trans*-4-Phenyl-3-buten-2-one	$C_6H_5CH{=}CHCOCH_3$	146.19	7, 364	1.0097_4^{45}	1.5836^{45}	41.5	260–262	65	v s alc, bz, chl, eth
p95	2-Phenyl-3-butyn-2-ol	$CH_3C(OH)(C_6H_5)C{\equiv}CH$	146.19	6^2, 559			47–49	217–218	96	0.8 aq; s alc, bz, acet
p96	3-Phenylbutyraldehyde	$CH_3CH(C_6H_5)CH_2CHO$	148.21	7^1, 168	0.997	1.5179^{20}		94^{16mm}	96	
p97	2-Phenylbutyric acid	$CH_3CH_2CH(C_6H_5)CO_2H$	164.20	9^2, 356	1.055	1.5160^{20}	42–44	270–2	>110	s bz, eth
p98	2-Phenylbutyronitrile	$CH_3CH_2CH(C_6H_5)CN$	145.21	9, 541	0.974	1.5086^{20}		114^{15mm}	105	
p99	Phenyl chloroformate	$C_6H_5O_2CCl$	156.57	6, 159	1.248	1.5107^{20}		71^{9mm}	75	
p100	Phenyl dichloro-phosphate	$C_6H_5OP(O)Cl_2$	210.98	6, 179	1.412	1.5230^{20}		241–243	>110	

4-Phenoxybutyl bromide, b281
Phenylacetaldehyde dimethyl acetal, d516
N-Phenylacetamide, a18
2-Phenylacetoacetonitrile, a51
Phenylacetone, p147
α-Phenylacetophenone, d26
β-Phenylacrylic acid, c279
γ-Phenylallyl alcohol, c282
Phenylamine, a293
β(Phenylamino)phenol, h115
N-Phenylaniline, d760
o-Phenylanisole, m63
Phenylarsonic acid, b12
Phenylazoformic acid 2-phenylhydrazide, d746
N-Phenylbenzamide, b5
Phenylbenzene, b138
α-Phenylbenzenemethanamine, a159
Phenylbenzoic acid, b139
Phenylboric acid, b13
Phenyl bromide, b262
1-Phenylbutane, b521
2-Phenylbutane, b522
1-Phenyl-1,3-butanedione, b63
4-Phenyl-2-butanone, b77a
Phenyl cellosolve, p72
Phenyl chloride, c47
Phenylcyclohexane, c376
2-Phenylcinchoninic acid, p153
α-Phenyl-*o*-cresol, h116



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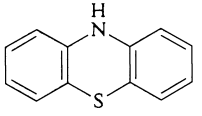

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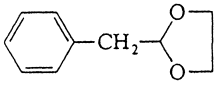

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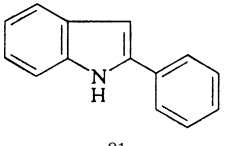

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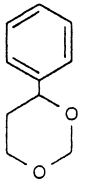
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
p101	*N*-Phenyldiethanol-amine	$C_6H_5N(CH_2CH_2OH)_2$	181.24	12, 183	1.120_{20}^{60}		56–80	350 sl dec		5 aq; v s alc; 29 eth; 25 bz
p102	4-Phenyl-1,3-dioxane		164.21	19[1], 616	1.111	1.5300^{20}		250–251	>110	
p103	2-Phenyl-1,3-dioxolane		150.18		1.106	1.5260^{20}		$80^{0.3mm}$	98	
p104	1,2-Phenylenediamine	C_6H_4-1,2-$(NH_2)_2$	108.14	13, 6			103	257		v s alc, chl, eth; sl s aq
p105	1,3-Phenylenediamine	C_6H_4-1,3-$(NH_2)_2$	108.14	13, 33	1.139^{15}		63.5	285		s aq, alc, acet, chl
p106	1,4-Phenylenediamine	C_6H_4-1,4-$(NH_2)_2$	108.14	13, 61			146	267	156	1 aq; s alc, chl, eth
p107	1,4-Phenylene diiso-cyanate	C_6H_4-1,4-$(NCO)_2$	160.13	13, 105			97–98	260	>110	
p108	1-Phenyl-1,2-ethanediol	$C_6H_5CH(OH)CH_2OH$	138.17	6, 907			66–68	272–274		v s aq, alc, bz, eth, chl, HOAc
p109	1-Phenylethanol	$CH_3CH(OH)(C_6H_5)$	122.17	6, 475	1.0130^{20}	1.5270^{20}	20	204	85	2.3 aq
p110	2-Phenylethanol	$C_6H_5CH_2CH_2OH$	122.17	6, 478	1.023_{25}^{25}	1.5317^{20}	−27	221	102	2 aq; misc alc, eth
p111	2-Phenylethyl acetate	$CH_3CO_2CH_2CH_2C_6H_5$	164.20	9, 510	0.984	1.4985^{20}		238–239	101	2 aq; misc alc, eth
p112	2-Phenylethylamine	$C_6H_5CH_2CH_2NH_2$	212.18	12, 1096	0.9640_4^{25}	1.5290^{25}	<0	197.5	90	80 aq[15]; s alc; i eth
p113	1-Phenylethyl propionate	$C_2H_5CO_2CH(CH_3)C_6H_5$	178.23	5[3], 1680	1.007	1.4895^{20}		92^{5mm}	94	
p114	(±)-2-Phenylglycine	$C_6H_5CH(NH_2)CO_2H$	151.17	14, 460			subl 255			s org solvents, alk
p115	1-Phenylheptane	$C_6H_5(CH_2)_6CH_3$	176.30	5, 451	0.860	1.4850^{20}		233	95	
p116	1-Phenylhexane	$C_6H_5(CH_2)_5CH_3$	162.28	5[2], 337	0.861	1.4860^{20}	−61	226	83	misc eth
p117	Phenylhydrazine	$C_6H_5NHNH_2$	108.14	15[2], 44	1.0978_4^{20}	1.6080^{20}	19.5	243	88	misc alc, bz, chl, eth
p118	Phenyl 1-hydroxy-2-naphthoate	$HOC_{10}H_6CO_2C_6H_5$	264.28	10, 332			94–96			
p119	Phenyl 3-hydroxy-2-naphthoate	$C_{10}H_6(OH)CO_2C_6H_5$	264.28	10, 335			129–132	261^{160mm}		
p120	2-Phenylimidazole		144.18	23, 182			144–147			
p121	2-Phenyl-2-imidazoline		146.19	23, 154			94–99			
p122	2-Phenyl-1,3-indandione		222.28	7, 808			148–150			
p123	2-Phenylindole		193.25	20, 467			188–190	250^{10mm}		
p124	Phenyl isocyanate	C_6H_5NCO	119.12	12, 437	1.0956_4^{20}	1.5350^{20}	−30	162–163	55	dec aq, alc; s eth
p125	Phenyl isothiocyanate	C_6H_5NCS	135.19	12, 453	1.1288_4^{25}	1.6497^{20}	−21	221	87	i aq; s alc, eth
p126	*N*-Phenylmaleimide		173.17	21, 400			85–87	163^{12mm}		s alc, chl, eth
p127	Phenylmalonic acid	$C_6H_5CH(CO_2H)_2$	180.16				153 dec			

p128	Phenylmercury(II) acetate	$C_6H_5HgO_2CCH_3$	336.74	Merck: 12, 7453			150–152			0.17 aq; s alc, bz, acet
p129	Phenylmercury(II) chloride	C_6H_5HgCl	313.15	Merck: 12, 7454			250–252			s bz, eth, pyr
p130	Phenylmercury(II) hydroxide	C_6H_5HgOH	294.70	16, 952			190 dec			
p131	*N*-Phenylmorpholine		163.22	27, 6	1.058^{270}		51–54	268	>110	1.0 aq; v s hot alc
p132	*N*-Phenyl-1-naphthylamine	$C_{10}H_7NHC_6H_5$	219.29	12, 1224			60–62	226^{15mm}		s alc, bz, chl, eth
p133	*N*-Phenyl-2-naphthylamine	$C_{10}H_7NHC_6H_5$	219.29	12, 1275			107–109	395		

Phenylethane, e74
Phenylethanenitrile, p82
1-Phenylethanol, m149
Phenylethanolamine, a257
N-Phenylethanolamine, a295
1-Phenylethanone, a31
Phenylethene, s11
N-Phenylformamide, f35
Phenylglyoxylic acid, b69
Phenylglyoxylonitrile, b67
2,2′-(Phenylimino)diethanol, p101
p-(2-Phenylisopropyl)phenol, m316a
Phenyl mercaptan, t156
Phenylmethanol, b78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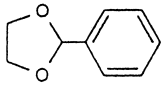
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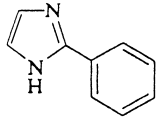
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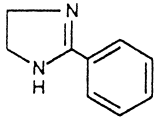
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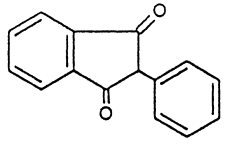
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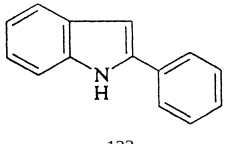
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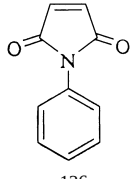
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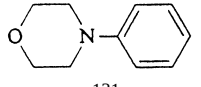
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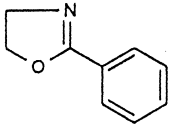
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
p134	2-Phenyl-2-oxazoline		147.18	27, 47	1.118	1.5670^{20}	12	$75^{0.3mm}$		
p135	2-Phenylphenol	$C_6H_5C_6H_4OH$	170.21	6^{2}, 623	1.213		57–59	282	123	s alc, chl, eth, alk
p136	4-Phenylphenol	$C_6H_5C_6H_4OH$	170.21	6, 674			165–167	321	165	s alc, chl, eth, alk
p137	*N*-Phenyl-1,4-phenylenediamine	$C_6H_5NHC_6H_4NH_2$	184.24	13, 76			73–75			
p138	Phenylphosphinic acid	$C_6H_5PH(O)OH$	142.09	16, 791			85–87			
p139	Phenylphosphonic acid	$C_6H_5P(O)(OH)_2$	158.09	16, 803			163–166			
p140	Phenylphosphonic dichloride	$C_6H_5P(O)Cl_2$	194.99	16, 804	1.375	1.5600^{20}	3	258	>110	
p141	*N*-Phenylpiperazine		162.24	23^{3}, 49	1.0621_4^{20}	1.5875^{20}		286	>110	i aq; misc alc
p142	1-Phenylpiperidine		161.25	20, 22	1.001	1.5620^{20}	3–4	257–258	106	
p143	2-Phenyl-1,2-propanediol	$CH_3C(C_6H_5)(OH)CH_2OH$	152.19	6, 930			44–45	162^{26mm}	>110	
p144	3-Phenyl-1-propanethiol	$C_6H_5CH_2CH_2CH_2SH$	152.26	6^{1}, 253	1.010	1.5494^{20}		109^{10mm}	90	
p145	1-Phenyl-1-propanol	$C_6H_5CH(OH)CH_2CH_3$	136.19	6, 502	0.9915_4^{25}	1.5200^{20}		219	90	misc alc, bz
p146	3-Phenyl-1-propanol	$C_6H_5CH_2CH_2CH_2OH$	136.19	6, 503	1.008	1.5257^{20}	−18	235	109	s aq; misc alc, eth
p147	1-Phenyl-2-propanone	$C_6H_5CH_2COCH_3$	134.18	7^{2}, 233	1.0157_4^{20}	1.5160^{20}	27	100^{13mm}	84	v s alc, eth; misc bz
p148	2-Phenylpropion-aldehyde	$CH_3CH(C_6H_5)CHO$	134.18	7, 305	1.009_4^{20}	1.5175^{20}		202–205	76	i aq; s alc
p149	3-Phenylpropion-aldehyde	$C_6H_5CH_2CH_2CHO$	134.18	7, 304	1.019	1.5230^{20}		98^{12mm}	95	
p150	3-Phenylpropionic acid	$C_6H_5CH_2CH_2CO_2H$	150.18	9, 508	1.047_4^{100}		47–49	280	>110	0.6 aq; s bz, alc, chl, eth, HOAc, PE
p151	1-Phenyl-3-pyrazolidinone		162.19	24, 2			121–123			10 hot aq; s hot alc, alk, acid
p152	2-Phenylpyridine	$C_6H_5C_5H_4N$	155.20	20, 424	1.086	1.6332^{20}		268–270	>110	s alc, eth
p153	2-Phenyl-4-quinoline-carboxylic acid		249.27	22, 103			214–215			0.8 alc; 1 eth; 0.3 chl
p154	Phenyl salicylate	$C_6H_5(OH)CO_2C_6H_5$	214.22	10, 76	1.25		44–46	173^{12mm}	>110	17 alc; 66 bz; s acet, chl, eth; 0.015 aq
p155	Phenylsuccinic acid	$HO_2CCH_2CH(C_6H_5)CO_2H$	194.19	9, 865			167–169	$-H_2O$, >168		s hot aq, alc, eth

p156	(Phenylthio)acetic acid	$C_6H_5SCH_2CO_2H$	168.21	6, 313			64–66			
p157	*S*-Phenyl thio-isobutyrate	$(CH_3)_2CHC(=O)SC_6H_5$	152.22	6,*4*, 1524	1.056	1.5460^{20}		129^{10mm}	>110	
p158	1-Phenyl-2-thiourea	$C_6H_5NHC(S)NH_2$	152.22	12, 388	1.3		154			0.25 aq; s alc, alk
p159	Phenyltrichlorosilane	$C_6H_5SiCl_3$	211.55	16, 911	1.329^{20}	1.5230^{20}		201	91	
p160	Phenyltriethoxysilane	$C_6H_5Si(OC_2H_5)_3$	240.38	16, 911	0.996	1.4604^{20}		113^{10mm}	42	
p161	Phenyltrimethoxy-silane	$C_6H_5Si(OCH_3)_3$	198.30	16^4, 1556	1.062	1.4680^{20}		233	99	
p162	Phenyltrimethyl-ammonium bromide	$[C_6H_5N(CH_3)_3]^+ Br^-$	216.13	12, 158			215 dec			v s aq; s hot alc
p163	Phenyltrimethyl-ammonium chloride	$[C_6H_5N(CH_3)_3]^+ Cl^-$	171.67	12, 158			237 subl			s aq; v s alc; sl s eth
p164	Phenyltrimethyl-ammonium iodide	$[C_6H_5N(CH_3)_3]^+ I^-$	263.12	12, 159			227 subl			s aq, alc; sl s acet
p165	Phenyltrimethyl-ammonium tribro-mide	$[C_6H_5N(CH_3)_3]^+ Br_3^-$	375.95	12, 159			114–116			
p166	Phenyltrimethylsilane	$C_6H_5Si(CH_3)_3$	150.30	16^1, 525	0.873	1.4907^{20}		168–170	44	
p167	Phenylurea	$C_6H_5NHCONH_2$	136.15	12, 346	1.302		145–147	238		s hot aq, hot alc, eth

1-Phenylpentane, p55
2-Phenylpropane, i103
3-Phenyl-2-propenoic acid, e279
3-Phenyl-2-propen-1-ol, c282
3-Phenyl-2-propenoyl chloride, c280
3-Phenylpropyl alcohol, p146
Phenyl propyl ketone, b619
3-Phenylpropyl mercaptan, p144
Phenyl sulfide, d770
Phenyl sulfone, d771
Phenylsulfonic acid, b23
Phenyl sulfoxide, d772
(Phenylthio)acetic acid, t157
Phenyl thiocarbamide, p158
α-Phenyl-*o*-toluic acid, b84
Phenyl *m*-tolyl ether, p76
Phloroglucinol, t318
Phorone, d613
Phthalaldehydic acid, f37



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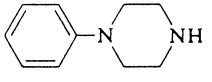

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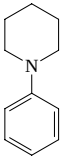

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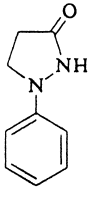

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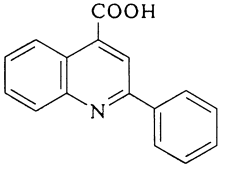

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TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
p168	1,2-Phthalic acid	C_6H_4-1,2-$(CO_2H)_2$	166.13	9, 791	1.593_4^{20}		230 rapid heating			0.6 aq; ;10 alc; 0.5 eth; v sl s chl
p169	Phthalic anhydride		148.12	17, 469	1.53		131–134	295	151	0.6 aq(dec); s alc
p170	Phthalide		134.13	17, 310	1.164_4^{99}		72–74	290		s alc
p171	Phthalimide		147.13	21, 458			234–236			v s alk; v sl s bz, PE
p172	1,2-Phthaloyl dichloride	C_6H_5-1,2-$(COCl)_2$	203.02	9, 805	1.409^{20}	1.5684^{20}	15–16	280–282	>110	dec by aq, alc; s eth
p173	Phthalylsulfathioazole		403.44	Merck: 12, 7533			272–277			s alk; sl s alc; i chl
p174	Picric acid	2,4,6-$(O_2N)_3C_6H_2OH$	229.11	6, 265	1.763_4^{20}		122–123	explodes >300		1.3 aq; 8.2 alc; 10 bz; 2.9 chl; 1.6 eth
p175	(+)-α-Pinene		136.24	5, 146	0.8591_4^{20}	1.4650^{20}	−62	156	35	misc alc, eth
p176	(−)-β-Pinene		136.24	5, 154	0.8590^{20}	1.4780^{20}	−61	166	38	
p177	α-Pinene oxide		152.24	5, 152	0.964	1.4690^{20}		103^{50mm}	65	
p178	Piperazine		86.14	23, 4		1.446^{113}	108–110	145–146	109	v s aq; 50 alc; i eth
p179	1,4-Piperazinebis-(ethanesulfonic acid)		302.37	Merck: 12, 7633			>300			
p180	Piperidine		85.15	20, 6	0.8622_4^{20}	1.4525^{20}	−13	106	4	misc aq; s alc, bz, chl
p181	1-Piperidinecarbo-nitrile		110.16	20, 56	0.951	1.4705^{20}		102^{10mm}	97	
p182	*N*-Piperidineethanol		129.20	20, 25	0.8732_{25}^{25}	1.4804^{20}		199–202	68	misc aq; s alc
p183	2-Piperidineethanol		129.20	21, 2	1.010^{17}		38–40	234	102	v s aq, alc, eth
p184	1-Piperidinepropionic acid		157.21	20[3], 1049			105–110	$108^{0.5mm}$		
p185	Piperidinepropionitrile		138.21		0.933	1.4695^{20}		111^{16mm}	102	
p186	2-(2-Piperidineethyl)-pyridine		190.29		0.985	1.5260^{20}		150^{17mm}	>110	
p187	L-Proline		115.13	22, 2			228 dec			

m-Phthalic acid, b17
p-Phthalic acid, b18
Phthalonitrile, d282

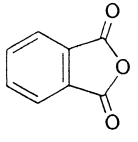
Pimelic ketone, c366
Pinacolone, d572
Pinacolyl alcohol, d571

Pivalic acid, d679
Pivalic anhydride, d680
Pivaloyl chloride, d681

Picolinaldehyde, p261
Picolines, m409 thru m411
Picolinic acids, p265, p267
Picolinonitrile, c328
Picolylamines, a218 thru a220
Picramide, t402
Pimelic acid, h7

Pipecolines, m381 thru m383
1-Piperazinoethanol, h129
1-Piperidinecarboxyaldehyde, f40
Piperonal, m250
Piperonyl butoxide, m252
cis-Piperylene, p16
Pivaldehyde, d677

Pivaloyloxymethyl chloride, c172
POPOP, b218
PPO, d779
Prehnitene, t97
Propadiene, a72
1-Propanal, p211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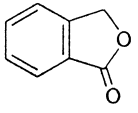
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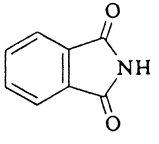
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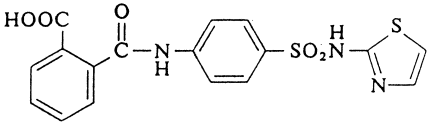
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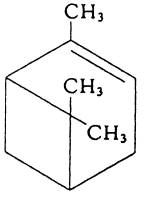
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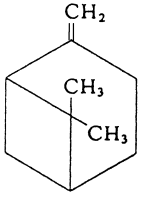
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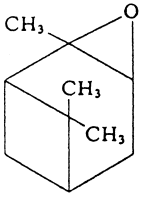
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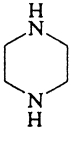
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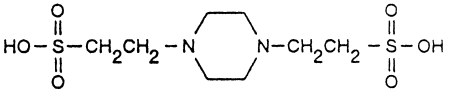
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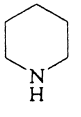
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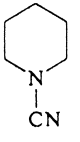
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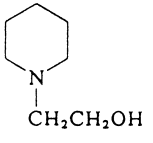
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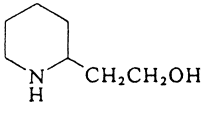
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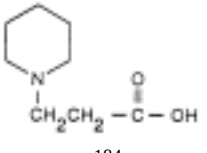
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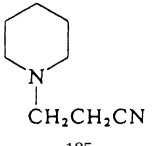
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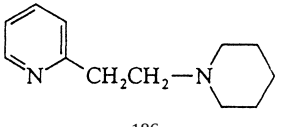
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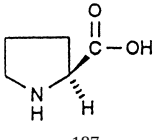
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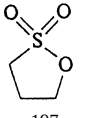
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
p188	Propane	$CH_3CH_2CH_3$	44.10	1, 103	0.584^{-42}	1.340^{-42}	−188	−42.1	−104	volumes per 100 vols solvent: 6.5 aq; 790 alc; 926 eth; 1300 chl; 1450 bz
p189	1,2-Propanediamine	$CH_3CH(NH_2)CH_2NH_2$	74.13	4, 257	0.878^{15}	1.4460^{20}		119–120	33	misc aq, bz; s alc, eth
p190	1,3-Propanediamine	$H_2NCH_2CH_2CH_2NH_2$	74.13	4, 261	0.884_4^{25}	1.4575^{20}	−12	140	48	misc alc, eth; s aq
p191	1,2-Propanediol	$CH_3CH(OH)CH_2OH$	76.10	1, 472	1.0364_4^{20}	1.4331^{20}	−60	188	107	misc aq, acet, chl; s alc, eth
p192	1,3-Propanediol	$HOCH_2CH_2CH_2OH$	76.10	1, 475	1.0538^{20}	1.4396^{20}	−27	214	79	misc aq, alc
p193	1,3-Propanediol bis-(4-aminobenzoate)	$CH_2(CH_2CO_2CC_6H_4NH_2)_2$	314.34	14^3, 1034	1.140		124–127			
p194	1,2-Propanediol dibenzoate	$C_6H_5CO_2CH_2CH(CH_3)$-$O_2CC_6H_5$	284.31	9, 129	1.160	1.5450^{20}	−3	232^{12mm}	>110	
p195	1,3-Propanedithiol	$HSCH_2CH_2CH_2SH$	108.23	1, 476	1.0772_4^{20}	1.5405^{20}	−79	172.9	58	misc alc, bz, eth, chl
p196	1-Propanesulfonyl chloride	$CH_3CH_2CH_2SO_2Cl$	142.60	4, 8	1.2864_4^{15}	1.4542^{20}		66^{8mm}	80	dec hot aq, hot alc
p197	1,3-Propane sultone		122.14	19^3, 4	1.392		31–33	180^{30mm}	>110	
p198	1-Propanethiol	$CH_3CH_2CH_2SH$	76.16	1, 359	0.836_4^{25}	1.4380^{20}	−113	67–68	−20	s alc, eth
p199	2-Propanethiol	$CH_3CH(SH)CH_3$	76.16	1, 367	0.809_4^{25}	1.4255^{20}	−131	52.6	−34	misc alc, eth; sl s aq
p200	1,2,3-Propanetriol tris(acetate)	$H_3CCO_2CH(CH_2O_2CCH_3)_3$	218.21	2, 147	1.1580^{20}	1.4302^{20}	−78	259	138	7.2 aq; misc alc, bz, chl, eth
p201	1-Propanol	$CH_3CH_2CH_2OH$	60.10	1, 350	0.8037^{20}	1.3840^{20}	−127	97.2	23	misc aq, alc, eth
p202	2-Propanol	$(CH_3)_2CHOH$	60.10	1, 360	0.7855_4^{20}	1.3772^{20}	−89.5	82.4	12	misc aq, alc, chl, eth
p203	2-Propenal	$H_2C{=}CHCHO$	56.07	1, 725	0.841_4^{20}	1.4017^{20}	−88	52.6	−18	21 aq; s alc, eth
p204	Propene	$H_2C{=}CHCH_3$	42.08	1, 196	0.610_4^{-48}	1.3567^{-40}	−185.2	−47.7	−108	vols in 100 vols solvent: 45 aq; 1200 alc; 500 acet
p205	2-Propene-1-thiol	$H_2C{=}CHCH_2SH$	74.15	1, 440	0.925_4^{23}	1.4765^{20}		67–68	21	misc alc, eth
p206	*trans*-1,2,3-Propene-tricarboxylic acid		174.11	2, 849			190 dec			50 aq[25]; 50 88% alc[12]; sl s eth
p207	1-Propen-2-yl acetate	$H_2C{=}C(O_2CCH_3)CH_3$	100.12		0.909	1.4000^{20}		97	18	

p208	4-(1-Propenyloxy-methyl)-1,3-dioxo-lan-2-one		158.16		1.100	1.4610^{20}		251–252	>110	
p209	2-Propenylphenol	$CH_3CH{=}CHC_6H_4OH$	134.18	6[1], 279	1.044	1.5780^{20}		230–231	90	
p210	*β*-Propiolactone		72.06	17[1], 130	1.1460_4^{20}	1.4131^{20}	−33.4	162	70	37 aq(hyd); misc alc (reacts); bz, eth, acet
p211	Propionaldehyde	CH_3CH_2CHO	58.08	1, 629	0.8071_4^{20}	1.3636^{20}	−81	48	−30	30 aq; misc alc, eth
p212	Propionamide	$CH_3CH_2CONH_2$	73.10	2, 243	0.9597_4^{80}	1.4160^{110}	79	222.2		v s aq, alc, chl, eth
p213	Propionic acid	$CH_3CH_2CO_2H$	74.09	2, 234	0.9934_4^{20}	1.3809^{20}	−20.5	141.1	52	misc aq; s alc, chl, eth
p214	Propionic anhydride	$[CH_3CH_2C(=O)]_2O$	130.14	2, 242	1.0110^{20}	1.4037^{20}	−45	170	63	dec aq; s alc, chl, eth
p215	Propionitrile	CH_3CH_2CN	55.08	2, 245	0.7818_4^{20}	1.3658^{20}	−92.8	97.2	2	10 aq; misc alc, eth
p216	Propionyl chloride	CH_3CH_2COCl	92.53	2, 243	1.065_4^{20}	1.4051^{20}	−94	80	11	dec by aq, alc
p217	Propiophenone	$C_6H_5COCH_2CH_3$	134.18	7[2], 231	1.0105_4^{20}	1.5258^{20}	21	218.0	87	misc bz, eth, abs alc
p218	2-Propoxyethanol	$CH_3CH_2CH_2OCH_2CH_2OH$	104.15	1, 468	0.913	1.4130^{20}	−75	150–153	48	
p219	2-(2-Propoxyethyl)-pyridine	$C_5H_4NCH_2CH_2OCH_2CH_2CH_3$	165.24		0.954	1.4880^{20}			95	
p220	1-Propoxy-2-propanol	$C_5H_4NCH_2CH_2OCH_2CH(OH)CH_3$	118.18	1[2], 536	0.885	1.4110^{20}		140–160	48	
p221	Propoxytrimethylsilane	$CH_3CH_2CH_2OSi(CH_3)_3$	132.28	4,*4*, 3994	0.768_4^{20}	1.3840^{20}		100^{735mm}	−2	
p222	Propyl acetate	$CH_3CH_2CH_2O_2CCH_3$	102.13	2, 129	0.8878	1.3844^{20}	−93	101.6	13	2.3 aq; misc alc, eth
p223	Propylamine	$CH_3CH_2CH_2NH_2$	59.11	4, 136	0.7173^{20}	1.3872^{20}	−83	42.2	−37	misc aq, alc, eth

1,3-Propanedicarboxylic acid, g14
Propanedioic acid, m3
1,2-Propanediol cyclic carbonate, p230
Propanenitrile, p215
1,2,3-Propanetriol, g19
Propanoic acid, p213
2-Propanone, a26
Propargyl alcohol, p249
Propargyl chloride, c241
Propenamide, a61
2-Propen-1-amine, a76
2-Propenenitrile, a63
3-Propenoic acid, a62
2-Propen-1-ol, a75
2-Propenyl acetate, a74
2-Propenylamine, a74
Propenylanisole, m107
N-2-Propenyl-2-propen-1-amine, d30
(2-Propenyl)thiourea, a97
Propiolic acid, p248
Propyl alcohol, p201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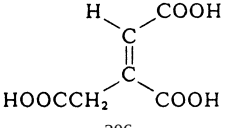
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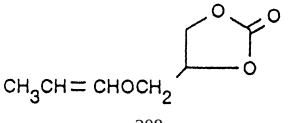
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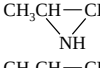
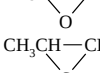
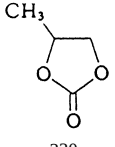
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
p224	2-(Propylamino)-ethanol	$C_3H_7NHCH_2CH_2OH$	103.17	4, 282	0.900	1.4415^{20}		182^{746mm}	78	
p225	Propylbenzene	$CH_3CH_2CH_2C_6H_5$	120.20	5, 390	0.8621_4^{20}	1.4912^{20}	−99.2	159.2	47	s alc, eth
p226	Propyl benzoate	$C_6H_5CO_2CH_2CH_2CH_3$	164.20	9, 112	1.032^{20}	1.5010^{20}	−51.6	230	98	i aq; s alc, eth
p227	Propyl butyrate	$CH_3CH_2CH_2CO_2CH_2CH_2CH_3$	130.19	2, 271	0.879_4^{15}	1.4000^{20}	−95	143	38	sl s aq; misc alc, eth
p228	Propyl chloroformate	$ClCO_2CH_2CH_2CH_3$	122.55	3, 11	1.090	1.4034^{20}		105–106	28	misc bz, chl, eth
p229	Propylcyclohexane	$CH_3CH_2CH_2C_6H_{11}$	126.24	5^2, 23	0.7929_4^{20}	1.4370^{20}	−94.9	156.7	35	s bz, eth
p230	Propylene carbonate		102.09	19^3, 1564	1.2041^{20}	1.4210^{20}	−48.8	242	135	v s aq, alc, bz, eth
p231	Propyleneimine		57.09	20, 3	0.8017^{25}	1.4084^{25}		66.0	−15	misc aq, alc, PE
p232	1,2-Propylene oxide		58.08	17, 6	0.8287^{20}	1.3660^{20}	−112	34	−35 (CC)	41 aq; misc alc, eth
p233	Propylene sulfide		74.15	17^2, 15	0.946	1.4760^{20}		72–75	10	
p234	Propyl formate	$CH_3CH_2CH_2O_2CH$	88.10	2, 21	0.9058^{20}	1.3779^{20}	−92.9	80.9	−3	2 aq; misc alc, eth
p235	Propyl 4-hydroxy-benzoate	$HOC_6H_4CO_2CH_2CH_2CH_3$	180.20	10, 160			95–98			0.05 aq; v s alc, eth
p236	Propyl isocyanate	$CH_3CH_2CH_2NCO$	85.11	4^1, 366	0.908	1.3940^{20}		83–84	0	
p237	Propyl lactate	$CH_3CH(OH)CO_2CH_2CH_2CH_3$	132.16	3, 265	0.996^{20}	1.4167^{25}		86^{40mm}		s aq, alc, eth
p238	Propyl nitrate	$CH_3CH_2CH_2ONO_2$	105.09	1, 355	1.0538_4^{20}	1.3976^{20}	−100	110.1	23 (may explode on heating)	s alc, eth
p239	2-Propylpentanoic acid	$(CH_3CH_2CH_2)_2CHCO_2H$	144.21	2, 350	0.921	1.4250^{20}		220	111	
p240	2-Propylphenol	$CH_3CH_2CH_2C_6H_4OH$	136.19	6, 499	1.015^{20}	1.5279^{20}		224–226	93	s alc, eth
p241	Propylphosphonic dichloride	$CH_3CH_2CH_2P(O)Cl_2$	160.97	4, 596	1.290	1.4643^{20}		90^{50mm}	>110	
p242	Propyltrichlorosilane	$CH_3CH_2CH_2SiCl_3$	177.53	4, 630	1.1851_4^{20}	1.429^{20}		123–124	2	
p243	1-Propyl-4-piperidone		141.22		0.936	1.4600^{20}		56^{1mm}	75	
p244	Propyl propionate	$CH_3CH_2CO_2CH_2CH_2CH_3$	116.16	2, 240	0.883^{20}	1.3935^{20}	−76	122.5	19	0.5 aq; 103 alc; 83 eth

p245	Propyl 3,4,5-trihydroxybenzoate	$(HO)_3C_6H_2CO_2CH_2CH_2CH_3$	212.20	Merck: 12, 8044			150			0.35 aq; 1 alc; 83 eth
p246	Propyne	$CH_3C{\equiv}CH$	40.06	1, 246	0.691^{-20}_{4}	1.3725^{-20}	−102.8	−23.2		v s alc; 3000 mL eth
p247	2-Propynyl benzenesulfonate	$C_6H_5SO_3CH_2C{\equiv}CH$	196.23	11^{3}, 37	1.243	1.5250^{20}	−30	142^{2mm}	100	
p248	2-Propynoic acid	$HC{\equiv}CCO_2H$	70.05	2, 477	1.138^{20}_{4}	1.4320^{20}	9	102^{200mm}	58	s aq, alc, eth
p249	2-Propyn-1-ol	$HC{\equiv}CH_2OH$	56.06	1, 454	0.9478^{20}	1.4320^{20}	−51.8	114	36	misc aq, alc, bz, chl
p250	(+)-Pulegone		152.24	7, 87	0.9346^{15}_{4}	1.4870^{20}		224	85	misc alc, chl, eth
p251	Pyrazine		80.09	23, 91	1.031^{61}_{4}	1.4953^{61}	55	115	55	v s aq, alc, eth
p252	Pyrazinecarbonitrile		105.10	25^{3}, 777	1.174	1.5340^{20}		87^{6mm}	96	
p253	Pyrazinecarboxylic acid		124.10	25, 125			225 dec			sl s hot aq; 0.008 abs alc; i bz, chl, eth
p254	Pyrazole		68.08	23, 39		1.4203	68	187		s aq, alc, bz, eth
p255	Pyrene		202.26	5, 693	1.271^{23}		151	404		s org solvents
p256	Pyridazine		80.09	23, 89	1.1035^{25}_{4}	1.5230^{23}	−8	208	85	misc aq, bz; v s alc, eth
p257	Pyridine	C_5H_5N	79.10	20, 181	0.9827^{25}_{4}	1.5067^{25}	−41.6	115.2	20	misc aq, alc, eth
p258	Pyridine-d_5	C_5D_5N	84.14	20^{3}, 2305	1.050	1.5092^{20}		114.4	20	
p259	2-Pyridinealdoxime	(C_5H_4N)-2-CH═NOH	122.13	21^{1}, 288			110–112			

Propyl bromide, b400
Propyl butanoate, p227
Propyl cyanide, b468a
Propyl chloride, c225
Propylene, p204
sec-Propylene chlorohydrin, c230
Propylene dibromide, d120
Propylenediamine, p189
Propylene glycol, p191
Propylene glycol dimethyl ether, d518
Propylene glycol monomethyl ether, m105
Propylene glycol monophenyl ether, p73
Propylene oxide, e15
Propyl gallate, p245
Propyl iodide, i48
Propyl mercaptan, p198
6-Propyl-2-thiouracil, h140
Pseudocumene, t358
Pyrene, b52
3,6-Pyridazinediol, d447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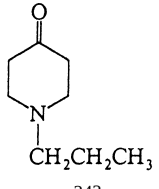
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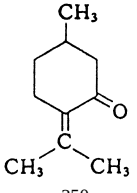
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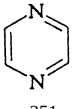
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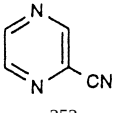
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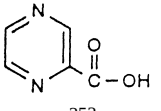
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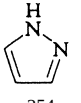
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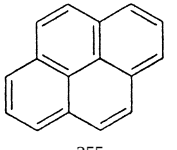
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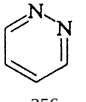
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TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
p260	4-Pyridinealdoxime	(C_5H_4N)-4-CH═NOH	122.13				130–133			
p261	2-Pyridinecarboxaldehyde	(C_5H_4N)-2-CHO	107.11	21^{1}, 287	1.126	1.5370^{20}		181	54	
p262	3-Pyridinecarboxaldehyde	(C_5H_4N)-3-CHO	107.11	21^{1}, 288	1.135	1.5493^{20}		97^{15mm}	60	
p263	4-Pyridinecarboxaldehyde	(C_5H_4N)-4-CHO	107.11	21, 287	1.122	1.5440^{20}		78^{12mm}	54	s aq, eth
p264	3-Pyridinecarboxamide	(C_5H_4N)-3-$CONH_2$	122.13	22, 40	1.400	1.466	130–133			100 aq; 66 alc
p265	2-Pyridinecarboxylic acid	(C_5H_4N)-2-CO_2H	123.11	22, 33			134–136	sublimes		s aq, alc, bz; v s HOAc
p266	3-Pyridinecarboxylic acid	(C_5H_4N)-3-CO_2H	123.11	22, 38	1.473		236.6	sublimes		1.4 aq; s alk; v s hot aq, hot alc
p267	4-Pyridinecarboxylic acid	(C_5H_4N)-4-CO_2H	123.11	22, 45			319	260^{15mm}		0.52 aq; i alc, bz, eth
p268	2,3-Pyridinedicarboxylic acid	(C_5H_4N)-2,3-$(CO_2H)_2$	167.12	22, 150			188–190 dec			0.56 aq; s alk
p269	2,5-Pyridinedicarboxylic acid	(C_5H_4N)-2,5-$(CO_2H)_2$	167.12	22, 153			256 dec			s hot acid
p270	2,6-Pyridinedicarboxylic acid	(C_5H_4N)-2,6-$(CO_2H)_2$	167.12	22, 154			248–250 dec			sl s aq; v sl s alc
p271	Pyridine-*N*-oxide	C_5H_5NO	95.10	20^{2}, 131			61–65	270		
p272	Pyridinium *p*-toluenesulfonate	$C_5H_5NH^+ \ ^-O_3SC_6H_4CH_3$	251.31	20^{2}, 129			117–119			
p273	2-Pyridylcarbinol	(C_5H_4N)-2-CH_2OH	109.13	21^{1}, 203	1.131	1.5420^{20}		113^{16mm}	>110	v s aq, alc, eth
p274	3-Pyridylcarbinol	(C_5H_4N)-3-CH_2OH	109.13	21, 50	1.124	1.5445^{20}		154^{28mm}	>110	v s aq, eth
p275	3-(3-Pyridyl)-1-propanol	(C_5H_4N)-3-$CH_2CH_2CH_2OH$	137.18	21^{3}, 549	1.063	1.5300^{20}		133^{3mm}	>110	
p276	3-(4-Pyridyl)-1-propanol	(C_5H_4N)-4-$CH_2CH_2CH_2OH$	137.18	21^{4}, 550	1.061		35–39	289	>110	
p277	Pyrimidine		80.09	23, 89	1.016	1.5040^{20}	22	124	31	misc aq; s alc, eth
p278	2,4(1*H*,3*H*)-Pyrimidinedione		112.09	24, 312			335			0.3 aq; s alk
p279	Pyrrole		67.09	20, 159	0.9691_4^{20}	1.5085^{20}	−23.4	130	39	4.5 aq; v s alc, eth
p280	Pyrrolidine		71.12	20, 4	0.8586^{20}	1.4431^{20}	−58	86.5	3	misc aq; s alc, chl, eth

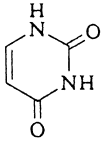
p281	1-Pyrrolidinebutyronitrile		138.21		0.926	1.4605^{20}		115^{18mm}	99	
p282	1-Pyrrolidinecarbodithioic acid, ammonium salt		164.29				153–155			
p283	1-Pyrrolidinecarbonitrile		96.13		0.954	1.4690^{20}		$77^{1.8mm}$	107	
p284	1-Pyrrolidino-1-cyclohexene		151.25		0.940	1.5225^{20}		115^{15mm}	39	
p285	2-Pyrrolidinone		85.11	21, 236	1.116_4^{25}	1.4806^{25}	25	251	129	misc aq, alc, bz, chl, eth, EtOAc
p286	3-(*N*-Pyrrolidino)-1,2-propanediol		145.20	20[1], 4			46–48	158^{30mm}	>110	

2,3-Pyridinediol, d448
2-Pyridineethanol, h132
3-Pyridinol *N*-oxide, h183
Pyridinols, h179 thru h181
2(1*H*)-Pyridone, h179
2-(2-Pyridyl)pyridine, d790

Pyrocatechol, d428
Pyrogallol, t317
Pyromellitic acid, b27
Pyromellitic dianhydride, b28
Pyromucic aldehyde, f44
Pyrrolidinedithiocarbamate, p282

1-Pyrrolidineethanol, h133
4-(*N*-Pyrrolidino)butyronitrile, p281
Pyruvic acid, o65
Pyruvic aldehyde, o64
Pyruvic aldehyde dimethyl acetal, d520


p277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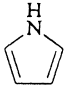
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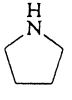
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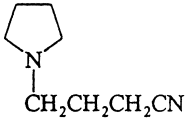
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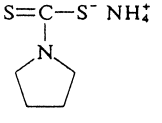
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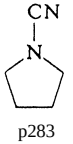
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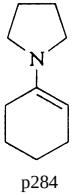
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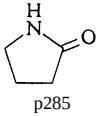
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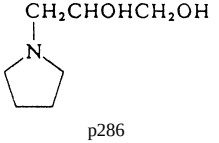
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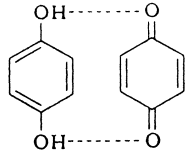
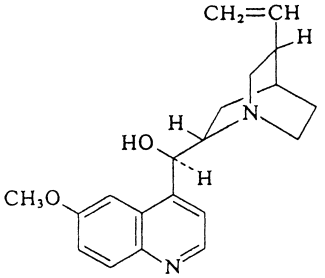
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
q1	Quinhydrone		218.20	7, 617	1.401_4^{20}		171–173			s hot aq, alc, eth
q2	Quinine		324.44	23, 511		1.625	173–175			125 alc; 1.2 bz; 83 chl
q3	Quinoline		129.16	20, 339	1.095_4^{20}	1.6273^{20}	−15	237	101	0.6 aq; misc alc, eth
q4	Quinoxaline		130.15	23, 176	1.334_4^{48}	1.6231^{48}	29–32	220–223	98	v s aq, alc, bz, eth
q5	2-Quinoxalinol		146.15	24, 147			271–272			
r1	**D**-Raffinose pentahydrate		594.52	31, 462			80–82	dec 118		14 aq; 10 MeOH
r2	Resorcinol	C_6H_4-1,3-$(OH)_2$	110.11	6, 796	1.272		110–112	280		111 aq; 111 alc; v s eth
r3	Resorcinol 1,3-diacetate	C_6H_4-1,3-$(O_2CCH_3)_2$	194.19	6, 816	1.178	1.5030^{20}		146^{12mm}	>110	
r4	Resorcinol monoacetate	$CH_3CO_2C_6H_4$-3-(OH)	152.15	6, 816	1.223	1.5370^{20}		*ca* 283	>110	i aq; misc alc, bz, chl, acet; s alk OH's
r5	Resorcinol monobenzoate	$C_6H_5CO_2C_6H_4$-3-(OH)	214.20					133–135		
r6	Rhodamine B		479.02	19, 345			210–211 dec			v s aq, alc
r7	Rhodanine		133.19	27, 242	0.868		167–170 may explode on rapid heating			v s hot aq, alc, eth
r8	Riboflavin		376.37	Merck: 12, 8367			dec 278–282			v s alk(dec); i acet, bz, eth; sl s pentyl acetate, cyclohexanol
r9	**D**-Ribose		150.13	1, 859			88–92			s aq; sl s alc
s1	Saccharin		183.19	27, 168	0.828		228–230			0.34 aq; 3 alc; 8 acet

Quinaldine, m420 *p*-Quinone, b58


q1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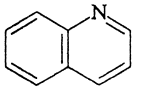
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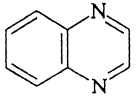
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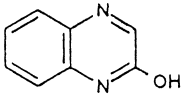
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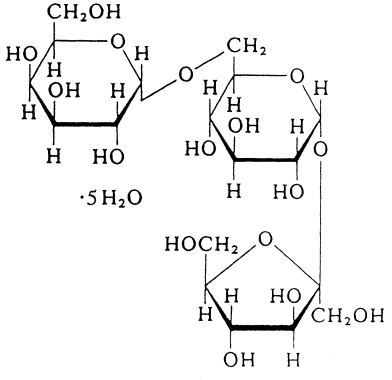
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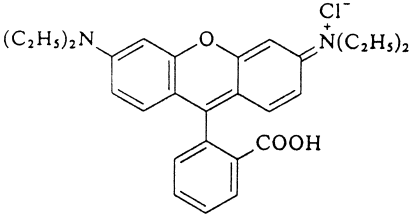
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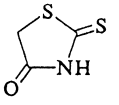
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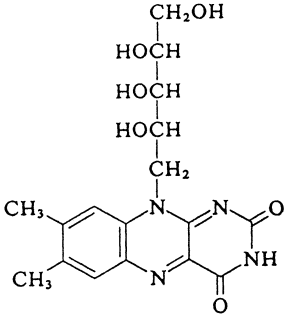
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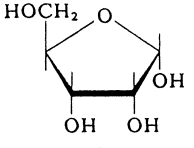
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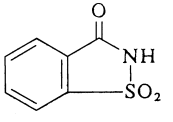
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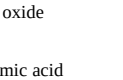
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

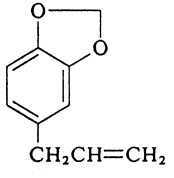
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
s2	Safrole		162.19	19, 39	1.095^{20}	1.5370^{20}	11.2	232–234	97	v s alc; misc chl, eth
s3	Semicarbazide hydrochloride	$H_2NNHCONH_2 \cdot HCl$	111.53	3, 98			175–177 dec			v s aq, alc; i eth
s4	**L**-Serine	$HOCH_2CH(NH_2)CO_2H$	105.09	4, 505			222 dec			s aq; v sl s alc, eth
s5	**D**-Sorbitol		182.17	1, 533	1.472^{-5}		98–100 if hydrated; 111 anhyd			83 aq; s hot alc, acet
s6	**L**-Sorbose		180.16	1, 927	1.65^{15}		163–165			55 aq; v sl s alc
s7	Squalane	$[(CH_3)_2CH(CH_3)_2CH(CH_3)$-$(CH_2)_3CH(CH_3)CH_2CH_2$-$]_2$	422.83	1[1], 72	0.8115^{15}	1.4530^{15}	−38	350	218	s bz, chl, eth, PE
s8	Squalene	$CH_3[C(CH_3)=CHCH_2CH_2]_5$-$C(CH_3)=C(CH_3)_2$	470.73	1[1], 130	0.8584_4^{20}	1.4965^{20}	−75	285^{25mm}	200	v s eth, acet, PE
s9	*trans*-Stilbene	$C_6H_5CH=CHC_6H_5$	180.25	5, 630	0.970		122–124	307		v s bz, eth
s10	(−)-Strychnine		334.42	27[2], 723	1.36_4^{20}		284–286	270^{5mm}		0.66 alc; 20 chl; 0.55 bz; 0.15 mg aq
s11	Styrene	$C_6H_5CH=CH_2$	104.15	5, 474	0.9060^{20}	1.5463^{20}	−31	145	31	s alc, acet, eth, CS_2
s12	Styrene oxide		120.15	17, 49	1.054	1.5338^{20}	−37	194	79	
s13	Succinamic acid	$H_2NCOCH_2CH_2CO_2H$	117.10	2, 614			153–156			s aq; sl s alc; i eth
s14	Succinamide	$H_2NCOCH_2CH_2CONH_2$	116.12	2, 614			265 dec			0.45 aq; i alc, eth
s15	Succinic acid	$HO_2CCH_2CH_2CO_2H$	118.09	2, 601	1.552		188	235 dec		7.7 aq; 5.4 alc; 2.8 acet; 0.88 eth; i bz
s16	Succinic anhydride		100.07	17, 407			119.6	261		s alc, chl; v sl s eth
s17	Succinimide		99.09	21, 369	1.41		123–125	285–290		33 aq; 4 alc; i eth
s18	Succinonitrile	$NCCH_2CH_2CN$	80.09	2, 615	0.9864^{60}	1.4173^{60}	54.5	266	132	*see* b456
s19	Succinyl chloride	$ClCOCH_2CH_2COCl$	154.98	2, 613	1.395_4^{15}	1.473^{15}	16–17	190	76	dec by aq, alc; s bz
s20	Sucrose		342.30	31, 424	1.587_4^{25}		185–187			200 aq; 0.59 alc
s21	Sulfadiazine		250.28	Merck: 12, 9071			252–256			sl s aq, alc, acet; v s dil mineral acids, alk
s22	Sulfamethazine		278.34	Merck: 12, 9083			198–201			0.15 aq; s alk

s23	Sulfamic acid	HSO_3NH_2	97.09	Merck: 12, 9090	2.15		205 dec			15 aq; sl s alc, acet; s bases
s24	Sulfanilamide	$H_2NC_6H_4SO_2NH_2$	172.21	14, 698			164–166			0.76 aq; 2.7 alc; 20 acet; s acid, alk
s25	Sulfanic acid	4-(H_2N)-$C_6H_4SO_3H$	173.19	14, 695			d 288			1.45 aq; sl s hot MeOH
s26	Sulfoacetic acid	$HCO_2CH_2SO_3H$	140.11	4, 21			84–86	245 dec		s aq, alc; i eth, chl
s27	2-Sulfobenzoic acid cyclic anhydride		184.17	19, 110				186^{18mm}		s bz, chl, eth; i aq

Salicylaldehyde, h94
Solketal, d599
Stearamide, o2
Stearic acid, o5
Stearyl bromide, b385

Stryene dibromide, d98
Stryene glycol, p108
Stryene oxide, e9
Suberic acid, o25
Suberonitrile, d285

Succinic acid monoamide, s13
Succinonitrile, b456
Sulfanilic acid, a117
Sulfolane, t107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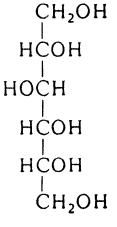
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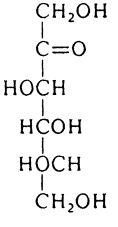
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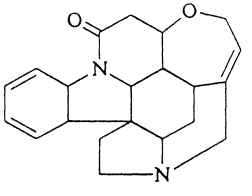
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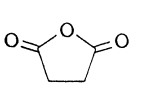
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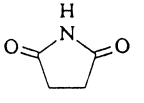
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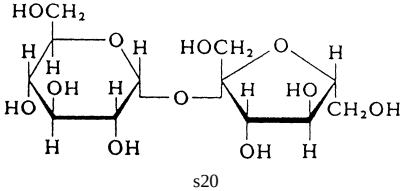
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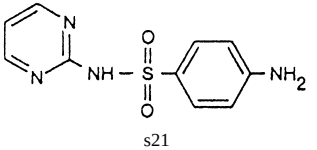
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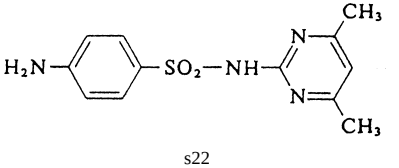
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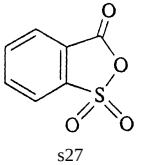
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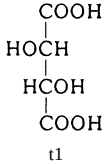
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
s28	4,4′-Sulfonylbis(2,6-dibromophenol)	$[2,6\text{-}(Br)_2—C_6H_2OH]_2SO_2$	565.88	6, 865			303–306			
s29	4,4′-Sulfonylbis(methyl benzoate)	$(CH_3O_2CC_6H_4)_2SO_2$	334.35	10^2, 109			195–196			
s30	4,4′-Sulfonyldiphenol	$(HOC_6H_4)_2SO_2$	250.27	6, 861	1.3663^{15}		245–247			s alc, eth, acet; i aq
s31	5-Sulfosalicylic acid	$HO_3SC_6H_3(OH)CO_2H$	254.21	11, 411			120 anhyd			v s aq, alc; s eth
t1	**D**-(−)-Tartaric acid		150.09	3, 520	1.7598^{20}_4		172–174			139 aq^{20}; 59 MeOH; 33 EtOH; s glyc; 0.4 eth
t2	**L**-(+)-Tartaric acid		150.09	3, 481	1.7598^{20}_4		168–170			139 aq^{20}; 59 MeOH; 33 EtOH; s glyc; 0.4 eth
t3	*meso*-Tartaric acid monohydrate	$HO_2CCH(OH)CH(OH)\text{-}CO_2H \cdot H_2O$	168.11	3, 528	1.666^{20}_4; 1.737 also		140; also 159–160			125 aq^{20}
t4	**DL**-Tartaric acid monohydrate	$HO_2CCH(OH)CH(OH)\text{-}CO_2H \cdot H_2O$	168.11	3, 522	1.697^{20}_4		210–212			20.6 aq^{20}; 5 alc^{25}; 1 eth
t5	Tartrazine		534.37	25, 252						v s aq
t6	Terephthaldicarbox-aldehyde	$C_6H_4\text{-}1,4\text{-}(CHO)_2$	134.13	7, 675			115–116	245–248		
t7	*m*-Terphenyl	$C_6H_5—C_6H_4—C_6H_5$	230.31	5, 695	1.195		87	363		
t8	*o*-Terphenyl	$C_6H_5—C_6H_4—C_6H_5$	230.31	5^2, 611	1.16		56.2	332	>110	
t9	*p*-Terphenyl	$C_6H_5—C_6H_4—C_6H_5$	230.31	5, 695	1.213		210	376	>110	
t10	α-Terpinene		136.24	5, 126	0.8375^{20}_4	1.4775^{20}		174	46	misc alc, eth
t11	γ-Terpinene		136.24	5, 128	0.853^{15}_4	1.4754^{16}		183	51	
t12	Terpinen-4-ol		154.25	6, 55	0.9338^{20}_4	1.4820^{20}	36.4	90^{6mm}	79	v s alc, eth
t13	α-Terpineol		154.25	6, 57	0.9337^{20}	1.4813^{20}	40.5	220	90	
t14	1,2,4,5-Tetrabromo-benzene	$C_6H_2Br_4$	393.72	5, 214			180–182			
t15	3,4,5,6-Tetrabromo-cresol	$CH_3C_6Br_4(OH)$	423.75	6, 362			205–208			s alc, eth, alk
t16	1,1,2,2,-Tetrabromo-ethane	$Br_2CHCHBr_2$	345.67	1, 94	2.9655^{20}	1.6358^{20}	0	243.5	none	misc alc, chl, eth, HOAc

t17	Tetrabromophthalic anhydride		463.72	17, 485			274–276			sl s bz; i aq, alc
t18	$\alpha,\alpha,\alpha',\alpha'$-Tetrabromo-*o*-xylene	C_6H_4-1,2-$(CHBr_2)_2$	421.77	5, 367			114–116			v s chl
t19	$\alpha,\alpha,\alpha',\alpha'$-Tetrabromo-*m*-xylene	C_6H_4-1,3-$(CHBr_2)_2$	421.77	5, 375			105–108			
t20	$\alpha,\alpha,\alpha',\alpha'$-Tetrabromo-*p*-xylene	C_6H_4-1,4-$(CHBr_2)_2$	421.77	5, 386			254–256			
t21	Tetrabutylammonium bromide	$(C_4H_9)_4N^+\ Br^-$	322.38	4[2], 634			102–104			
t22	Tetrabutylammonium chloride	$(C_4H_9)_4N^+\ Cl^-$	277.92	4[3], 292			73–75			
t23	Tetrabutylammonium hydrogen sulfate	$(C_4H_9)_4N^+\ HSO_4^-$	339.54				171–173			
t24	Tetrabutylammonium iodide	$(C_4H_9)_4N^+\ I^-$	369.38	4, 157			145–147			sl s aq; s alc, eth
t25	Tetrabutylammonium tetrafluoroborate	$(C_4H_9)_4N^+\ BF_4^-$	329.28	4[3], 293			160–162			
t26	Tetrabutylammonium tribromide	$(C_4H_9)_4N^+\ Br_3^-$	482.20	4[4], 557			74–76			

Sulfonyldianiline, d47, d48
Sylvan, m259
Sylvic acid, a1
2,4,5-T, t246
Taurine, a160
Terephthalaldehyde, b14
Terephthaldicarboxaldehyde, b14
Terephthalic acid, b18
Terephthaloyl chloride, b16
Tetrabromomethane, c13
Tetrabutoxysilane, t28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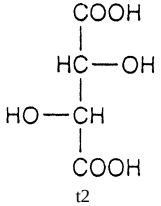
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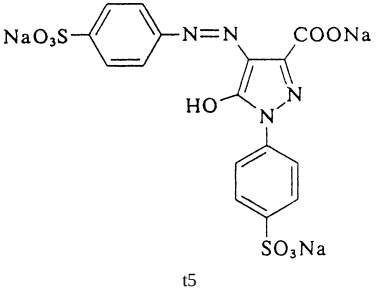
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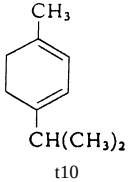
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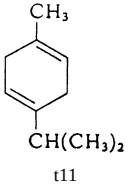
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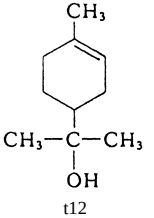
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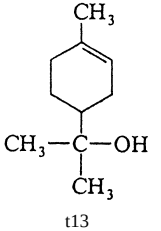
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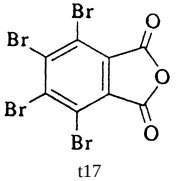
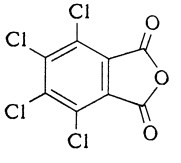

t17

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
t27	*N,N,N′,N′*-Tetrabutyl-1,6-hexanediamine	$\{\text{-}(CH_2)_3N[(CH_2)_3]_2\}_2$	340.64		0.820	1.4510^{20}		83^{2mm}	57	
t28	Tetrabutyl orthosilicate	$Si[O(CH_2)_3CH_3]_4$	320.55	1^2, 398	0.899_4^{20}	1.4131^{20}		275	78	
t29	Tetrabutyl phosphonium bromide	$[CH_3(CH_2)_3]_4PBr$	339.35				100–103			
t30	Tetrabutyltin	$(C_4H_9)_4Sn$	347.15		1.057	1.4742^{20}	−97	145^{10mm}	107	
t31	1,1,3,3,-Tetrachloroacetone	$Cl_2CHC(=O)CHCl_2$	195.86	1, 656	1.624_4^{15}	1.497^{18}		182^{745mm}	none	v s acet, chl
t32	1,2,3,4-Tetrachlorobenzene	$C_6H_2Cl_4$	215.89	5, 204			46–47	254	>110	v s eth; sl s alc
t33	1,2,4,5-Tetrachlorobenzene	$C_6H_2Cl_4$	215.89	5, 205	1.858^{22}		139–142	240–246	>110	s bz, chl, eth
t34	Tetrachloro-1,2-benzoquinone	C_6Cl_4-1,2-$(=O)_2$	245.88	7, 602			127–129			
t35	Tetrachloro-1,4-benzoquinone	C_6Cl_4-1,4-$(=O)_2$	245.88	7, 636			290 dec			s eth; sl s chl; i aq
t36	Tetrachloro-1,2-difluoroethane	$Cl_2CFCFCl_2$	203.83		1.6447^{25}	1.4130^{25}	26.0	92.8		0.012 aq
t36a	1,1,1,2-Tetrachloroethane	$ClCH_2CCl_3$	167.85	1, 86	1.5406^{20}	1.4821^{20}	−70.2	130.5	47	
t37	1,1,2,2-Tetrachloroethane	$Cl_2CHCHCl_2$	167.85	1, 86	1.5866_4^{25}	1.4910^{25}	−44	147	62	0.3 aq; misc alc, chl, eth, PE
t38	Tetrachloroethylene	$Cl_2C{=}CCl_2$	165.83	1, 187	1.6230_4^{20}	1.5057^{20}	−22	121	45	misc alc, chl, eth
t39	2,3,5,6-Tetrachloronitrobenzene	$HC_6Cl_4NO_2$	260.89	5, 247	1.744_4^{25}		98–101	304		s alc, bz, chl
t40	Tetrachlorophthalic anhydride		285.90	17, 484			254–258	371		dec hot aq; sl s eth
t41	Tetracosane	$CH_3(CH_2)_{22}CH_3$	338.66	1, 175	0.7786^{51}	1.4283^{70}	51	391	>110	9.4 chl; s eth
t42	Tetradecafluorohexane	$CF_3(CF_2)_4CF_3$	338.05	1^3, 388	1.669	1.2515^{20}	−4	58–60	none	
t43	Tetradecane	$CH_3(CH_2)_{12}CH_3$	198.40	1, 171	0.7627_4^{20}	1.4290^{20}	5.5	253.6	99	v s alc, eth
t44	Tetradecanoic acid	$CH_3(CH_2)_{12}CO_2H$	228.38	2, 365	0.8525_4^{70}	1.4273^{70}	54	250^{100mm}		v s bz, chl, eth; s alc
t45	1-Tetradecanol	$CH_3(CH_2)_{13}OH$	214.39	1, 428	0.8151^{50}	1.4358^{50}	39.5	289	>110	s eth; sl s alc
t46	Tetradecanoyl chloride	$CH_3(CH_2)_{12}COCl$	246.82	2, 368	0.908	1.4490^{20}	−1	168^{15mm}	>110	dec aq, alc; s eth

t47	1-Tetradecene	$CH_3(CH_2)_{11}CH{=}CH_2$	196.38	1, 226	0.775_4^{15}	1.4360^{20}	−12.9	251.2	115	v s alc, eth
t48	Tetraethoxysilane	$(CH_3CH_2O)_4Si$	208.33	1, 334	0.934_4^{20}	1.383^{20}	−77	168	46	dec aq; s alc
t49	Tetraethylammonium bromide	$(CH_3CH_2)_4N^+\ Br^-$	210.16	4, 104	1.397_4^{20}		285 dec			v s aq, alc, acet, chl
t50	Tetraethylammonium chloride	$(CH_3CH_2)_4N^+\ Cl^-$	165.71	4, 104	1.0801_4^{21}					141 aq; s alc; 8.2 chl
t51	Tetra(ethylene glycol)	$(HOCH_2CH_2OCH_2CH_2)_2O$	194.23	1, 468	1.125_{20}^{20}	1.4577^{20}	−6	328	182	misc aq, alc, bz, eth
t52	Tetra(ethylene glycol) diacrylate	$(H_2C{=}CHCO_2CH_2CH_2O\text{-}CH_2CH_2)_2O$	302.33		1.110	1.4650^{20}			>110	
t53	Tetra(ethylene glycol) diethyl ether	$C_2H_5(OCH_2CH_2)_4OC_2H_5$	250.34	1[3], 2107	0.970	1.4324^{20}		159^{11mm}	>110	s aq
t54	Tetra(ethylene glycol) dimethacrylate	$[H_2C{=}C(CH_3)CO_2CH_2CH_2\text{-}OCH_2CH_2]_2O$	330.37	2[4], 1531	1.080	1.4630^{20}		220	>110	
t55	Tetra(ethylene glycol) dimethyl ether	$CH_3(OCH_2CH_2)_4OCH_3$	222.28	1[3], 2107	1.0087_4^{20}	1.4330^{20}	−30	275–276	140	s aq
t56	Tetraethylene-pentamine	$(H_2NCH_2CH_2NHCH_2CH_2)_2NH$	189.31	4,*3*, 543	0.999_{20}^{20}	1.5055^{20}	−40	340	185	misc aq, alc, eth
t57	*N,N,N′,N′*-Tetraethyl-ethylenediamine	$(C_2H_5)_2NCH_2CH_2N(C_2H_5)_2$	172.32	4, 251	0.808	1.4343^{20}		189–192	58	
t58	Tetraethylgermanium	$(C_2H_5)_4Ge$	188.84	4, 631	0.998	1.4420^{20}	−90	165.5	35	s alc, eth; i aq
t59	Tetraethyllead	$(C_2H_5)_4Pb$	323.45	4, 639	1.653_4^{20}	1.5190^{20}	−136	85^{15mm}	72	s bz; misc eth
t60	Tetraethylsilane	$(C_2H_5)_4Si$	144.34	4, 625	0.7658^{20}	1.4268^{20}	−82	154.7	26	i aq
t61	*N,N,N′,N′*-Tetraethyl-sulfamide	$(C_2H_5)_2NSO_2N(C_2H_5)_2$	208.33	4, 129	1.030	1.4480^{20}		249–251	>110	

Tetracene, b7
Tetrachloromethane, c14
α,α,α,2-Tetrachlorotoluene, c58
α,α,α,4-Tetrachlorotoluene, c59
Tetradecyl alcohol, t45
Tetraethylmethane, d386a
Tetraethyl orthosilicate, t48



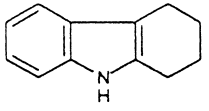
t40

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
t62	Tetraethylthiuram disulfide	$[(C_2H_5)_2NC(=S)S^-]_2$	296.54	4, 122	1.30		71–72			3.8 alc; 7.1 eth; s bz, acet, chl; 0.02 aq
t63	Tetraethyltin	$(C_2H_5)_4Sn$	234.94	4, 632	1.199^{20}	1.4730^{20}	−112	181	53	i aq; s eth
t64	1,1,1,2-Tetrafluoroethane	FCH_2CF_3	102.03	1,*4*, 123			−26.5			
t65	Tetrafluoroethylene	$F_2C{=}CF_2$	100.02	1[3], 638	1.151^{-40}		−142.5	−76		i aq
t66	2,2,3,3-Tetrafluoro-1-propanol	$HCF_2CF_2CH_2OH$	132.06	1[4], 1438	1.4853_4^{20}	1.3197^{20}	−15	109–110	43	
t67	1,2,3,6-Tetrahydrobenzaldehyde	C_6H_9CHO	110.16	7[1], 48	0.940	1.4745^{20}		163–164	57	
t68	1,2,3,4-Tetrahydrocarbazole		171.24	20, 416			118–120	325–330		
t69	Tetrahydrofuran		72.11	17, 10	0.8892_4^{20}	1.4052^{20}	−108.5	65	−14	misc aq, alc, eth, PE
t70	2,5-Tetrahydrofuran-dimethanol		132.16		1.1542_4^{25}	1.4766^{25}	<-50	265		misc aq, alc, bz, chl; s eth
t71	Tetrahydro-2-furanmethanol		102.13	17[2], 106	1.0524^{20}	1.4520^{20}	<-80	178	75	misc aq, alc, bz, chl, eth, acet
t72	Tetrahydro-2-furanmethylamine		101.15	18[2], 415	0.980	1.4560^{20}		154^{744mm}	45	
t73	Tetrahydrofurfuryl acetate		144.17	17[2], 107	1.061	1.4370^{20}		196	84	
t74	Tetrahydrofurfuryl acrylate		156.18	17[3], 1104	1.064	1.4600^{20}		87^{9mm}	>110	
t75	Tetrahydrofurfuryl chloride		120.58	17[3], 61	1.110	1.4550^{20}		150–151	47	
t76	Tetrahydrofurfuryl methacrylate		170.21	17[3], 1105	1.044	1.4580^{20}		$52^{0.4mm}$	90	
t77	2(3)-(Tetrahydrofuryloxy)tetrahydropyran		186.25		1.030	1.4610^{20}			97	
t78	1,2,3,4-Tetrahydroisoquinoline		133.19	20, 275	1.064	1.5668^{20}	−30	232–233	98	
t79	Tetrahydrolinalool	$(CH_3)_2CHCH_2CH_2CH_2$-$C(CH_3)(OH)CH_2CH_3$	158.29	1, 426	0.826	1.4340^{20}	76	73^{6mm}	76	

t80	1,2,3,4-Tetrahydro-naphthalene	$C_{10}H_{12}$	132.21	5, 491	0.9702_4^{20}	1.5414^{20}	−35.8	207.6	77	misc alc, bz, chl, eth, acet, PE
t81	*cis*-1,2,3,6-Tetrahydro-phthalic anhydride		152.15	17, 462			97–103		157	
t82	*cis*-1,2,3,6-Tetrahydro-phthalimide		151.17				129–133			
t83	Tetrahydropyran		86.14	17, 12	0.8814_4^{20}	1.4200^{20}	−45	88	−155	misc aq, alc, eth

Tetraethyl titanate(IV), t163
Tetrafluoromethane, c15
Tetraglyme, b212
1,2,3,4-Tetrahydrobenzene, c368
Tetrahydrodicyclopentadiene, t259
Tetrahydro-2,5-dimethoxyfuran, d525
Tetrahydrofurfuryl alcohol, t70
Tetrahydrofurfuralamine, t72
Tetrahydrolinalool, d668
Tetrahydro-2-methylfuran, m429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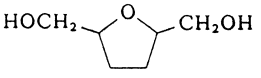
t69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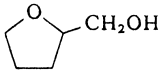
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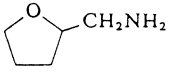
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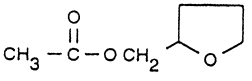
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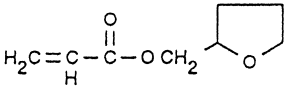
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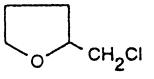
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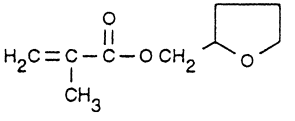
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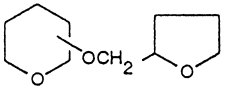
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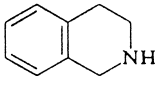
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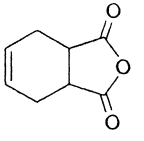
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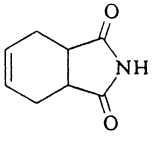

t82

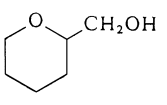

t83

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
t84	Tetrahydropyran-2-methanol		116.16		1.0254^{20}	1.4580^{20}	−70	187	93	misc aq, alc, bz, eth
t85	3,4,5,6-Tetrahydropyrimidinethiol		116.19	24, 5			210–212			
t86	1,2,3,4-Tetrahydroquinoline		133.19	20, 262	1.061	1.5940^{20}	15–16	249	100	s aq; misc alc, eth
t87	Tetrahydrothiophene		88.17	17[1], 5	0.9987^{20}	1.5040^{20}	−96	121	12	misc alc, eth; i aq
t88	2,2′,4,4′-Tetrahydroxybenzophenone	$[(HO)_2C_6H_3]_2C{=}O$	246.22	8, 496			200–203			
t89	Tetrakis(dimethylamino)ethylene	$[(CH_3)_2N]_2C{=}C[N(CH_3)_2]_2$	200.23	4[4], 167	0.861	1.4800^{20}		$59^{0.9mm}$	53	
t90	*N*,*N*,*N*′,*N*′-Tetrakis(2-hydroxypropyl)-ethylenediamine	$[CH_3CH(OH)CH_2]_2NCH_2$-$CH_2N[CH_2CH(OH)CH_3]_2$	292.40	4[4], 1685	1.013	1.4812^{20}		$181^{0.8mm}$	>110	
t91	1,1,8,8-Tetramethoxyoctane	$(CH_3O)_2CH(CH_2)_6CH(OCH_3)_2$	234.34		0.949	1.4300^{20}		130^{5mm}	52	
t92	1,1,3,3-Tetramethoxypropane	$[(CH_3O)_2CH]_2CH_2$	164.20		0.997	1.4081^{20}		183	54	
t93	Tetramethylammonium bromide	$(CH_3)_4N^+\ Br^-$	154.06	4, 51	1.56		>300			55 aq
t94	Tetramethylammonium chloride	$(CH_3)_4N^+\ Cl^-$	109.60	4, 51	1.169_4^{20}		>300			s aq, hot alc
t95	Tetramethylammonium iodide	$(CH_3)_4N^+\ I^-$	201.06	4, 51	1.829		>300			sl s aq; v s abs alc
t96	*N*,*N*-3,5-Tetramethylaniline	$(CH_3)_2C_6H_3N(CH_3)_2$	149.24	12, 1131	0.913	1.5443^{20}		226–228	90	
t97	1,2,3,4-Tetramethylbenzene	C_6H_2-1,2,3,4-$(CH_3)_4$	134.22	5, 430	0.905_4^{20}	1.5187^{20}	−6.2	205.0	68	misc alc, eth
t98	1,2,3,5-Tetramethylbenzene	C_6H_2-1,2,3,5-$(CH_3)_4$	134.22	5, 430	0.8906_4^{20}	1.5134^{20}	−23.7	198.0	63	s alc; v s eth
t99	1,2,4,5-Tetramethylbenzene	C_6H_2-1,2,4,5-$(CH_3)_4$	134.22	5, 431	0.838_4^{81}		79.3	196.8	73	v s alc, bz, eth
t100	2,2,3,3-Tetramethylbutane	$(CH_3)_3CC(CH_3)_3$	114.23	1, 165	0.8242^{20}		−100.7	106.5	4	

t101	*N,N,N′,N′*-Tetramethyl-1,3-butanediamine	$(CH_3)_2NCH(CH_3)CH_2CH_2N(CH_3)_2$	144.26	4^3, 570	0.787	1.4318^{20}		165	40	
t102	*N,N,N′,N′*-Tetramethyl-1,4-butanediamine	$(CH_3)_2N(CH_2)_4N(CH_3)_2$	144.26	4, 265	0.786^{20}	1.4280^{20}		169	46	s aq, alc, eth
t103	1,1,3,3-Tetramethylbutylamine	$(CH_3)_3CCH_2C(CH_3)_2NH_2$	129.25	4, 198	0.805	1.4240^{20}		137–143	32	s alc, eth, PE; i aq
t104	1,3,5,7-Tetramethylcyclotetrasiloxane	$[-SiH(CH_3)O-]_4$	240.51	4^4, 4099	0.9912_4^{20}	1.3870^{20}	−69	134–135		
t105	*N,N,N′,N′*-Tetramethyldiaminomethane	$(CH_3)_2NCH_2N(CH_3)_2$	102.18	4, 54	0.749	1.4005^{20}		85	−12	
t106	1,1,3,3-Tetramethyldisiloxane	$[(CH_3)_2CH]_2O$	134.33	4^4, 3991	0.757_4^{20}	1.3700^{20}		70–71	−10	
t107	Tetramethylene sulfone		120.17	17^1, 5	1.2606_4^{30}	1.4820^{30}	27.6	285	177	misc aq, acet, toluene; s octanes, olifines, naphthenes
t108	*N,N,N′,N′*-Tetramethylethylenediamine	$(CH_3)_2NCH_2CH_2N(CH_3)_2$	116.21	4, 250	0.770	1.4179^{20}	−55	120–122	10	
t109	Tetramethylgermanium	$(CH_3)_4Ge$	132.73	4,*2*, 1008	0.978	1.3890^{20}	−88	43.4	−37	
t110	1,1,3,3-Tetramethylguanadine	$[(CH_3)_2N]_2C{=}NH$	115.18	4^1, 335	0.918	1.4692^{20}		163	60	

Tetrahydropyrrole, p280
6,7,8,9-Tetrahydro-5*H*-tetrazolazepine, p27
Tetrahydrothiophene 1,1-dioxide, t107
Tetraiodomethane, c16
Tetralin, t80
β-Tetralonehydantoin, b40
N,N,N′,N′-Tetramethyldiaminomethane, t113
N,N,N′,N′-Tetramethyl-1,3-diamino-2-propanol, b180
2,2,5,5-Tetramethyl-3,4-dithiahexane, d171
Tetramethylene, c333
Tetramethyl glycol, b457
Tetramethylene oxide, t69
Tetramethylene sulfide, t87
Tetramethylethylene glycol, d569



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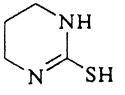

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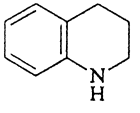

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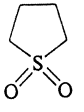
t87



t107

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

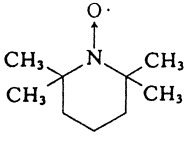
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
t111	*N,N,N′,N′*-Tetramethyl-1,6-hexanediamine	$[(CH_3)_2N(CH_2)_3-]_2$	172.32	4[1], 423	0.806	1.4359^{20}		209–210	73	
t112	Tetramethyl lead	$(CH_3)_4Pb$	267.33	4, 639	1.995^{20}_4		−27.5	110	38	misc alc, eth
t113	*N,N,N′,N′*-Tetramethylmethanediamine	$(CH_3)_2NCH_2N(CH_3)_2$	102.18	4, 54	0.749	1.4005^{20}		85	−12	
t114	2,6,10,14-Tetramethylpentadecane	$[(CH_3)_2CH(CH_3)_3-CH(CH_3)CH_2]_2CH_2$	268.53	Merck: 12, 7932	0.7827^{20}_4	1.4385^{20}	−100	296	>110	s bz, chl, eth, PE
t115	2,2,6,6-Tetramethylpiperidinyl-1-oxy (free radical)		156.25				36–40		67	
t116	*N,N,N′,N′*-Tetramethyl-1,3-propanediamine	$(CH_3)_2N(CH_2)_3N(CH_3)_2$	130.24	4, 262	0.779	1.4234^{20}		145–146	31	
t117	Tetramethylpyrazine		136.20	23, 99			84–86	190		
t118	Tetramethylsilane	$(CH_3)_4Si$	88.23	4, 625	0.6411^{20}_4	1.3580^{20}	−99.5	26.5	−27	v s alc, eth
t119	1,1,3,3-Tetramethyl-2-thiourea	$(CH_3)_2NC(=S)N(CH_3)_2$	132.23	4[1], 336			75–77	245		0.002 alc, 0.002 eth; 0.012 acet; 0.025 bz; s chl
t120	Tetramethylthiuram disulfide	$[(CH_3)_2NCS_2-]_2$	240.43	4, 76	1.29		155–156			
t121	Tetramethyltin	$(CH_3)_4Sn$	178.83	4, 631	1.3149^{25}	1.5201	−54	74–75	−12	
t122	1,1,3,3-Tetramethylurea	$(CH_3)_2NC(=O)N(CH_3)_2$	116.16	4, 74	0.9687^{20}_4	1.4493^{25}	−0.6	176–177	77	misc aq, common org solvents
t123	Tetranitromethane	$C(NO_2)_4$	196.03	1, 80	1.6229^{25}_4	1.4358^{25}	13.8	126	>110	v s alc, eth, alk
t124	1,4,7,10-Tetraoxacyclododecane (12-Crown-4)		176.21		1.089	1.4630^{20}	16	$70^{0.5mm}$	>110	
t125	2,4,8,10-Tetraoxaspiro[5.5]undecane		160.17	19, 436			52–55	$83^{1.5mm}$	108	
t126	Tetraphenylboron sodium	$(C_6H_5)_4B^-\ Na^+$	342.23	Merck: 12, 8839			>300			v s aq, acet; s chl

t127	1,1,4,4-Tetraphenyl-1,3-butadiene	$(C_6H_5)_2C{=}CHCH{=}C(C_6H_5)_2$	358.49	5, 750			207–209			
t128	Tetraphenyltin	$(C_6H_5)_4Sn$	427.11		1.490^{0}		224–227	>420	110	
t129	Tetrapropoxysilane	$(C_3H_7O)_4Si$	264.4	1, 355	0.916_4^2	1.401^{20}		94^{5mm}	95	
t130	Tetrapropylammonium bromide	$(CH_3CH_2CH_2)_4N^+\ Br^-$	266.27	4^1, 364			270 dec			s aq
t131	1*H*-Tetrazole		70.06	26, 346			157–158			s aq, alc, acet
t132	2-Thenoyltrifluoro-acetone		222.18				40–44	98^{8mm}		
t133	Theobromine		180.17	26, 457			357	sublimes 290–295		100 aq; 0.045 alc; s alk; i bz, chl, eth

Tetramethylolmethane, p19
2,2,4,4-Tetramethyl-3-thiapentane, d147
Tetramethylthiuram disulfide, b183

Tetrantoin, b40
2,5,8,13-Tetraoxododecane, b211
Tetraphene, b6

Tetrapropoxytitanate(IV), t163
2-Thenoic acid, t155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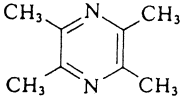
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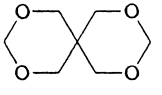
t124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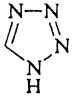
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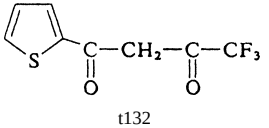
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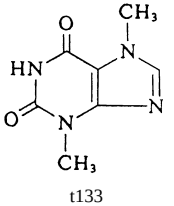
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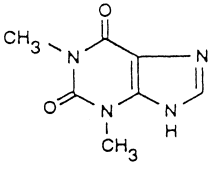
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
t134	Theophylline		180.17	26, 455			274–275			0.83 aq; 1.25 alc; 0.9 chl; s hot aq, alk, dil acids
t135	Thiamine HCl		337.27	Merck: 12, 9430			dec 260			100 aq; 1 alc; 5.5 glyc
t136	Thiazole		85.13	27, 15	1.200	1.5390^{20}		117–118	22	s alc, eth; sl s aq
t137	N^2-(2-Thiazolyl)-sulfanilamide		255.32	27^3, 4623			202			0.06 aq; 0.52 alc; s acet, dil mineral acids, alkalis
t138	Thioacetamide	$CH_3C(=S)NH_2$	75.13	2, 232			112–114			16 aq; 16 alc; sl s eth
t139	Thiobenzoic acid	$C_6H_5C(=O)SH$	138.19	9, 419	1.174	1.6050^{20}	15–18	122^{30mm}	>110	misc eth; v s alc; i aq
t140	4,4′-Thiobis(2-*tert*-butyl-6-methyl-phenol)		358.54	6^4, 6043			163–165	316^{40mm}	240	
t141	Thiocarbanilide	$C_6H_5NHC(=S)NHC_6H_5$	228.32	12, 394	1.32^{24}		152–155			v s alc, eth
t142	*p*-Thiocresol	$HSC_6H_4CH_3$	124.21	6, 416			42–44	195	68	s alc, eth; i aq
t143	2,2′-Thiodiacetic acid	$(HO_2CCH_2)_2S$	150.15	3, 253			128–131			s aq, alc
t144	2,2′-Thiodiethanol	$(HOCH_2CH_2)_2S$	122.19	1, 470	1.1824_4^{20}	1.5203^{20}	−10.2	282	160	misc aq, alc; sl s eth
t145	4,4′-Thiodiphenol	$(HOC_6H_4)_2S$	218.27	6, 860			154–156			
t146	3,3′-Thiodipropionic acid	$(HO_2CCH_2CH_2)_2S$	178.21				131–134			3.7 aq; v s hot aq, alc, acet
t147	Thiolacetic acid	$CH_3C(=O)SH$	76.12	2, 230	1.065	1.4630	< −17	88–91	11	s aq; v s alc
t148	*N*-Thionylaniline	$C_6H_5N=SO$	139.18	12, 578	1.236	1.6270^{20}		200	84	
t149	Thionyl bromide	$SOBr_2$	207.88	Merck: 12, 9484	2.683	1.6750^{20}	−52	138		misc bz, chl, CCl_4; hyd by aq
t150	Thionyl chloride	$SOCl_2$	118.97	Merck: 12, 9485	1.635	1.517^{20}	−101	76	none	misc bz, chl, CCl_4; hyd by aq
t151	Thiophene	C_4H_4S	84.14	17, 29	1.0573_4^{25}	1.5257^{25}	−39.4	84	−1	misc alc, eth; i aq
t152	2-Thiopheneacetic acid	$(C_4H_3S)CH_2CO_2H$	142.18	18, 293			63–67	160^{22mm}		
t153	2-Thiophenecarbonyl chloride	$(C_4H_3S)COCl$	146.60	18, 290	1.371	1.5900^{20}		206–208	90	
t154	2-Thiophenecarbox-aldehyde	$(C_4H_3S)CHO$	112.15	17, 285	1.200	1.5900^{20}		198	77	s eth

t155	2-Thiophenecarboxylic acid	$(C_4H_3S)CO_2H$	128.15	18, 289			127–130	260		s aq, chl; v s alc, eth
t156	Thiophenol	C_6H_5SH	110.18	6, 294	1.073	1.5880^{20}	−14.9	169	50	v s alc; misc bz, eth
t157	Thiophenoxyacetic acid	$C_6H_5SCH_2CO_2H$	168.21	6, 313			64–66			
t158	Thiophosphoryl chloride	$PSCl_3$	169.40		1.668	1.5550^{20}	−36 (β) −40 (α)	125	none	s bz, chl, CCl_4, CS_2

2-Thiabutane, e221
Thiacyclopentane, t87
1,3,4-Thiadiazole-2,5-dithiol, d486
3-Thiaheptane, b557
2-Thiahexane, b577
3-Thiahexane, e255
Thianaphthene, b60
5-Thianonane, d170
2-Thiapentane, m406
3-Thiapentane, d398
Thioanisole, m379
2-Thiobarbituric acid, d437
1,1′-Thiobis(butane), d170
Thiocarbanilide, d791
2,2′-Thiodiethanethiol, b209
Thiodiethylene glycol, t144
Thiodiglycol, t144
Thiodiglycolic acid, t143
Thioethanol, e26a
Thioethanolamine, a161
1-Thioglycerol, m21
Thioglycolic acid, m16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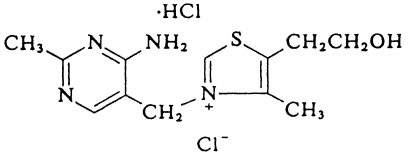
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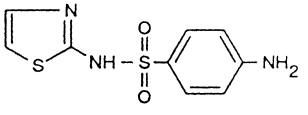
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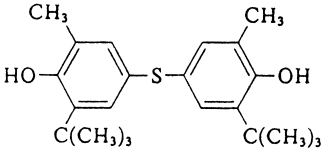
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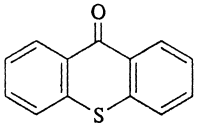
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

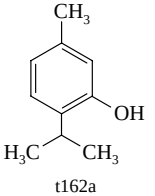
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
t159	Thiopropionic acid	$CH_3CH_2C(=O)SH$	90.14	2, 264	1.014	1.4640^{20}		108–110	11	
t160	3-Thiosemicarbazide	$H_2NC(=S)NHNH_2$	91.14	3, 195			182–184			s aq, alc
t161	Thiourea	$H_2NC(=S)NH_2$	76.12	3, 180	1.405		176–178			9 aq; s alc; sl s eth
t162	Thioxanthen-9-one		212.27	17, 357			212–213	373^{715mm}		v s bz, chl, hot HOAc
t162a	Thymol		150.22	6, 532	0.9699^{25}_{4}	1.5227^{20}	51.5	233	102	0.1 aq; 100 alc; 140 eth; s HOAc, alk OH
t163	Titanium(IV) ethoxide	$Ti(OC_2H_5)_4$	228.15	1, 335	1.088	1.5043^{20}		152^{10mm}	28	
t164	Titanium(IV) isopropoxide	$Ti[OCH(CH_3)_2]_4$	284.26	1^2, 382	0.963	1.4660^{20}	18–20	220	22	s bz, chl, eth
t165	Titanium(IV) propoxide	$Ti(OCH_2CH_2CH_3)_4$	284.26	1^3, 1423	1.033	1.4986^{20}		170^{3mm}	42	
t166	Toluene	$C_6H_5CH_3$	92.14	5, 280	0.8660^{20}_{4}	1.4960^{20}	−94.9	110.6	4	misc alc, chl, eth, acet, HOAc; 0.067 aq
t167	2,4-Toluenediamine	$CH_3C_6H_3$-2,4-$(NH_2)_2$	122.17	13, 124			99	292		s hot aq, alc, eth
t168	2,5-Toluenediamine	$CH_3C_6H_3$-2,5-$(NH_2)_2$	122.17	13, 144			64	273–274		v s aq, alc, eth
t169	2,6-Toluenediamine	$CH_3C_6H_3$-2,6-$(NH_2)_2$	122.17	13, 148			104–106			s aq, alc
t170	3,4-Toluenediamine	$CH_3C_6H_3$-3,4-$(NH_2)_2$	122.17	13, 148			91–93	156^{18mm}		v s aq
t171	Toluene-2,4-diisocyanate	$CH_3C_6H_3$-2,4-$(NCO)_2$	174.16	13, 138	1.2244^{20}_{4}	1.5689^{20}	20–21	251	132	dec aq, alc; misc acet, bz, eth
t172	*p*-Toluenesulfinic acid	$CH_3C_6H_4SO_2H$	156.21	11, 9			85			v s alc, eth; sl s aq
t173	*o*-Toluenesulfonamide	$CH_3C_6H_4SO_2NH_2$	171.22	11, 86			156–158			
t174	*p*-Toluenesulfonamide	$CH_3C_6H_4SO_2NH_2$	171.22	11, 104			138–140			0.2 aq; 3.6 alc
t175	*p*-Toluenesulfonylhydrazide	$CH_3C_6H_4SO_2NHNH_2$	186.23	11^2, 66			110 dec			
t176	*p*-Toluenesulfonic acid	$CH_3C_6H_4SO_3H$	172.20	11, 97			107 anhyd	140^{20mm}		67 aq; s alc, eth
t177	*p*-Toluenesulfonyl chloride	$CH_3C_6H_4SO_2Cl$	190.65	11, 103			67–69	134^{10mm}		v s alc, bz, eth; i aq
t178	*p*-Toluenesulfonyl fluoride	$CH_3C_6H_4SO_2F$	174.19	11^2, 54			41–42	112^{16mm}	105	

t179	*p*-Toluenesulfonyl isocyanate	$CH_3C_6H_4SO_2NCO$	197.21			1.4355^{20}		144^{10mm}	>110	
t180	*m*-Toluidine	$CH_3C_6H_4NH_2$	107.16	12, 853	0.989_4^{20}	1.5680^{20}	−31	203	85 (CC)	misc alc, eth
t181	*o*-Toluidine	$CH_3C_6H_4NH_2$	107.16	12, 772	0.998^{20}	1.5720^{20}	−16.3	200	85	1.7 aq; s alc, eth
t182	*p*-Toluidine	$CH_3C_6H_4NH_2$	107.16	12, 880	0.9619^{20}	1.5532^{59}	43.8	200	87	7.4 aq; v s alc, eth
t183	*m*-Tolunitrile	$CH_3C_6H_4CN$	117.15	9, 477	0.976^{15}	1.5256^{20}	−23	210	86	0.09 aq; v s alc, eth
t184	*o*-Tolunitrile	$CH_3C_6H_4CN$	117.15	9, 466	0.989	1.5279^{20}	−13	205	84	i aq; misc alc, eth
t185	*p*-Tolunitrile	$CH_3C_6H_4CN$	117.15	9, 489	0.9785_4^{30}		29.5	217	85	i aq; v s alc, eth
t186	2-(*p*-Toluoyl)benzoic acid	$CH_3C_6H_4COC_6H_4CO_2H$	240.26	10, 759			137–139			v s alc, bz, eth, acet
t187	*m*-Toluoyl chloride	$CH_3C_6H_4COCl$	154.60	9, 477	1.173	1.5485^{20}		86^{5mm}	76	
t188	*o*-Toluoyl chloride	$CH_3C_6H_4COCl$	154.60	9, 464	1.185	1.5549^{20}		90^{12mm}	76	
t189	*p*-Toluoyl chloride	$CH_3C_6H_4COCl$	154.60	9, 484	1.169	1.5530^{20}	−2	225–227	82	
t190	*p*-Tolyl acetate	$CH_3CO_2C_6H_4CH_3$	150.18	6, 397	1.048	1.5010^{20}		210–211	90	
t191	1-(*o*-Tolyl)biguanide	$CH_3C_6H_4NHC(=NH)NHC(=NH)NH_2$	191.24	12^3, 1873			143–145		>110	
t192	*m*-Tolyl isocyanate	$CH_3C_6H_4NCO$	133.15	12, 864	1.033	1.5305^{20}		76^{12mm}	65	s alc, eth; i aq
t193	1,2,4-Triacetoxybenzene	$C_6H_3(O_2CCH_3)_3$	252.22	6, 1089			98–100			
t194	Triacetoxyvinylsilane	$(CH_3CO_2)_3SiCH=CH_2$	232.26		1.167	1.4220^{20}		128^{25mm}	76	
t195	Triallylamine	$(H_2C=CHCH_2)_3N$	137.23	4, 208	0.790	1.4510^{20}	150–151		30	

Thiolactic acid, m22
Thiomalic acid, m25
Thiosalicylic acid, m18
Thiosinamine, a97
2-Thioxo-4-thiazolidinone, r7
Threonine, a185
Tiglic acid, m169
Tioxolone, h105
TMS, t118
TMSi, t396
Tolan, d742
p-Tolualdehyde, m138
Toluenethiol, t142
Toluic acids, m142 thru 144
α-Tolunitrile, p82
p-Tolylacetamide, m374
Tolyl bromide, b431
α-Tolyl chloride, b90
Tolyl chlorides, c255 thru c257



t162



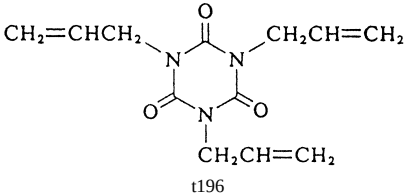
t162a

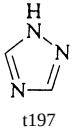
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
t196	Triallyl-1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione		249.27		1.159	1.5129^{20}		152^{4mm}	>110	
t197	1*H*-1,2,4-Triazole		69.07	26, 13			119–121	260		s aq, alc
t198	Tribenzylamine	$(C_6H_5CH_2)_3N$	287.41	12, 1038	0.991_4^{95}		91–94		65	s hot alc, eth
t199	Tribromoacetaldehyde	Br_3CCHO	280.76	1, 626	2.665	1.5850^{20}		174	65	s aq, alc, chl, eth
t200	Tribromoacetic acid	Br_3CCO_2H	296.76	2, 220			130–133	245		s aq, alc, eth
t201	2,4,6-Tribromoaniline	$Br_3C_6H_2NH_2$	329.83	12, 663	2.35		120–122	300		s hot alc, chl, eth
t202	2,2,2-Tribromoethanol	Br_3CCH_2OH	282.77	1^2, 338			73–79	93^{10mm}		2 aq; s alc, bz, eth
t203	1,1,2-Tribromo-ethylene	$BrCH{=}CBr_2$	264.74	1, 191	1.708^{21}	1.6247^{25}		162.5		
t204	Tribromomethane	$CHBr_3$	252.77	1, 68	2.9000^{15}	1.6005^{15}	8.1	149.6	83	0.3 aq; misc eth, MeOH
t205	2,4,6-Tribromophenol	$Br_3C_6H_2OH$	330.82	6, 203	2.55		87–89	290^{746mm}		s alc, chl, eth; i aq
t206	1,2,3-Tribromopropane	$BrCH_2CH(Br)CH_2Br$	280.78	1, 112	2.390	1.584^{18}	16.5	220	93	s alc, eth
t207	Tributoxyborane	$(C_4H_9O)_3B$	230.16	1^2, 398	0.8567^{20}	1.4092^{20}	< −70	234	93	hyd aq
t208	Tributylamine	$(C_4H_9)_3N$	185.36	4, 157	0.7784	1.4280^{20}	−70	216	86	v s alc, eth; s acet
t209	Tributylborane	$(C_4H_9)_3B$	182.16	4^2, 1022	0.747			109^{20mm}	−36	i aq; s most org solv
t210	2,4,6-Tri-*tert*-butyl-phenol	$[(CH_3)_3C]_3C_6H_2OH$	262.44		0.864_4^{27}		129–132	277		
t211	Tributyl phosphate	$(C_4H_9O)_3P(O)$	266.32	1^2, 397	0.9727^{25}	1.4226^{25}	−79	289	146	0.04 aq; misc org solv
t212	Tributyl phosphite	$(C_4H_9O)_3P$	250.32	1^1, 187	0.925_4^{20}	1.4326^{20}		125^{7mm}	91	misc alc, bz, eth, PE
t213	Tributyltin chloride	$(C_4H_9)_3SnCl$	325.49	4^3, 1926	1.200	1.4905^{20}		173^{25mm}	>110	
t214	Tributyltin ethoxide	$(C_4H_9)_3SnOC_2H_5$	335.10		1.098	1.4672^{20}		$92^{0.1mm}$	40	
t215	Tributyltin hydride	$(C_4H_9)_3SnH$	291.05	4^4, 4312	1.082	1.4730^{20}		$80^{0.4mm}$	40	
t216	Tributyltin methoxide	$(C_4H_9)_3SnOCH_3$	321.07	4^4, 4331	1.115	1.4720^{20}		$97^{0.06mm}$	98	
t217	Trichloroacetamide	Cl_3CCONH_2	162.40	2, 211			141–143	238–240		
t218	Trichloroacetaldehyde	Cl_3CCHO	147.40	Merck: 12, 9755	1.510_4^{20}	1.4557^{20}	−57.5	97.8		dec aq, alc; s eth
t219	Trichloroacetic acid	Cl_3CCO_2H	163.39	2, 206	1.629_4^{61}	1.6200^{20}	57.5	196.5	>110	120 aq; v s alc, eth
t220	Trichloroacetic anhydride	$(Cl_3CCO)_2O$	308.75	2, 210	1.690	1.4838^{20}		141^{60mm}	none	
t221	1,1,3-Trichloroacetone	$ClCH_2COCHCl_2$	161.42	1, 655	1.508	1.4892^{20}	13–15	172	79	
t222	Trichloroacetonitrile	Cl_3CCN	144.39	2, 212	1.4403_4^{25}	1.4409^{20}	−42	86	none	

t223	2,2′,4′-Trichloroacetophenone	$Cl_2C_6H_3COCH_2Cl$	223.49	7, 283			52–55	135^{4mm}	>110	
t224	Trichloroacetyl chloride	Cl_3CCOCl	181.83	2, 210	1.629	1.4689^{20}	−146	118		
t225	2,4,5-Trichloroaniline	$Cl_3C_6H_2NH_2$	196.46	12, 627			93–95	270		s alc
t226	2,4,6-Trichloroaniline	$Cl_3C_6H_2NH_2$	196.46	12, 627			73–75	262		s alc, eth
t227	1,2,3-Trichlorobenzene	$C_6H_3Cl_3$	181.45	5, 203	1.69	1.5776^{20}	53–55	218–220	126	v s bz, CS_2; sl s alc
t228	1,2,4-Trichlorobenzene	$C_6H_3Cl_3$	181.45	5, 204	1.454^{20}	1.5707^{20}	17	213–214	110	misc bz, eth, PE
t229	1,3,5-Trichlorobenzene	$C_6H_3Cl_3$	181.45	5, 204	1.66	1.5662^{19}	63.5	208	107	v s bz, eth, PE
t230	Trichloro-3-chloropropylsilane	$Cl(CH_2)_3SiCl_3$	211.98		1.350	1.4666^{20}		181–183		
t231	1,1,1-Trichloroethane	CH_3CCl_3	133.41	1, 85	1.3390^{20}	1.4379^{20}	−30.4	74	−1	s acet, bz, eth
t232	1,1,2-Trichloroethane	$ClCH_2CHCl_2$	133.41	1, 85	1.4397^{20}	1.4714^{20}	−37	114	32	misc alc, eth
t233	2,2,2-Trichloroethanol	Cl_3CCH_2OH	149.40	1, 338	1.557	1.4900^{20}	18	151–153		8 aq; misc alc, eth
t234	2,2,2-Trichloroethyl chloroformate	$ClCO_2CH_2CCl_3$	211.86		1.539	1.4703^{20}		171–172		
t235	Trichloroethylene	$ClCH{=}CCl_2$	131.39	1, 187	1.4642^{20}	1.4773^{20}	−84.8	87	32	0.1 aq; misc alc, chl, eth
t236	Trichloroethylsilane	$C_2H_5SiCl_3$	163.51	4, 630	1.2373^{20}	1.4256^{20}	−105.6	100.5	22	
t237	Trichlorofluoromethane	Cl_3CF	137.37	Merck: 12, 9770	1.485^{21}	1.384^{20}	−111	23.8		0.14 aq; s alc, eth
t238	α,α,2-Trichloro-6-fluorotoluene	$ClC_6H_3(F)CHCl_2$	213.47	5^3, 701	1.446	1.5506^{20}		228–230	>110	
t239	Trichloroisocyanuric acid		232.41	25, 256			249–251			

Triacetin, p200
1,3,5-Triazine-2,4,6-triol, c332
Tributyl borate, t207
Tributyrin, g20
Trichloroethanal, t218
β,β,β-Trichloroethoxycarbonyl chloride, t234


t196


t197

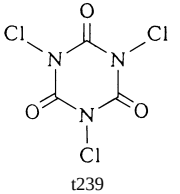

t239

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

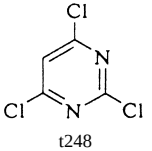
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
t240	Trichloromethane-sulfenyl chloride	Cl_3CSCl	185.89	3, 135	1.700_4^{20}	1.5436^{20}		146–148		
t241	1,1,1-Trichloro-2-methyl-2-propanol	$(CH_3)_2C(OH)CCl_3$	177.46	1, 382			99 anhyd	167		s alc, bz, chl, eth
t242	Trichloromethylsilane	CH_3SiCl_3	149.48	4^3, 1896	1.273_4^{20}	1.4108^{20}	−90	66	−9	
t243	1,2,4-Trichloro-5-nitrobenzene	$Cl_3C_6H_2NO_2$	226.45	5, 246	1.790^{20}		49–55	288	>110	v s bz, eth
t244	2,4,5-Trichlorophenol	$Cl_3C_6H_2OH$	197.45	6^2, 180			67–69	253		615 acet; 163 bz; 525 eth; 615 MeOH; i aq
t245	2,4,6-Trichlorophenol	$Cl_3C_6H_2OH$	197.45	6, 190	1.4901_4^{75}		69	246	none	525 acet; 113 bz; 354 eth; 525 MeOH; i aq
t246	(2,4,5-Trichloro-phenoxy)acetic acid	$Cl_3C_6H_2OCH_2CO_2H$	255.49	6^3, 702			154–158			s alc; v sl s aq
t247	1,2,3-Trichloropropane	$ClCH_2CH(Cl)CH_2Cl$	147.43	1, 106	1.3889^{20}	1.4854^{20}	−14.7	157	71	misc alc, eth; i aq
t248	2,4,6-Trichloro-pyrimidine		183.43	23, 90		1.5700^{20}	23–25	>110		
t249	Trichlorosilane	$HSiCl_3$	135.45	Merck: 12, 9776	1.342	1.4000^{20}	−127	31–32	−13	dec aq; s bz, chl
t250	4-(Trichlorosilyl)-butyronitrile	$Cl_3Si(CH_2)_3CN$	202.54	*4*,*4*, 4272	1.300	1.4630^{20}		237–238	92	
t251	α,α,α-Trichlorotoluene	$C_6H_5CCl_3$	195.48	5, 300	1.3723^{20}	1.5580^{20}	−5	219–223	127	s alc, bz, eth
t252	α,2,4-Trichlorotoluene	$Cl_2C_6H_3CH_2Cl$	195.48	5^4, 819	1.407	1.5760^{20}	−2.6	248	>110	
t253	α,2,6-Trichlorotoluene	$Cl_2C_6H_3CH_2Cl$	195.48			1.5761^{20}	36–39	119^{14mm}	>110	v s alc, eth
t254	α,3,4-Trichlorotoluene	$Cl_2C_6H_3CH_2Cl$	195.48	5, 300	1.411	1.5766^{20}		124^{14mm}	>110	
t255	2,4,6-Trichloro-1,3,5-triazine		184.41	26, 35			146–148	190		i aq; s alc
t256	1,1,1-Trichlorotri-fluoroethane	Cl_3CCF_3	187.38		1.579	1.3699^{20}	13–14	46		
t257	1,1,2-Trichlorotri-fluoroethane	$Cl_2CFCClF_2$	187.38	1^3, 157	1.5635^{25}	1.3557^{25}	−35	47.7		0.017 aq
t258	Trichlorovinylsilane	$H_2C{=}CHSiCl_3$	161.49		1.270	1.4360^{20}	−95	90	10	

t259	Tricyclo[5.2.1.0^{2,6}]-decane		136.24	5, 164			77–79	193	40	
t260	Tricyclo[5.2.1.0^{2,6}]-decan-8-one		150.22	7^{2}, 133	1.063	1.5025^{20}		132^{30mm}		
t261	Tridecane	$CH_3(CH_2)_{11}CH_3$	184.37	1, 171	0.7563$^{20}_{4}$	1.4256^{20}	−5 to −4	235	70	v s alc, eth
t262	Tridecanoic acid	$CH_3(CH_2)_{11}CO_2H$	214.35	2, 364			41–42	236^{100mm}	>110	v s alc, eth; i aq
t263	2-Tridecanone	$CH_3(CH_2)_{10}COCH_3$	198.35	1, 715	0.822	1.4350^{20}	29–31	134^{10mm}	>110	
t264	7-Tridecanone	$[CH_3(CH_2)_5]_2CO$	198.35	1, 715	0.825		30–32	264	>110	
t265	1-Tridecene	$CH_3(CH_2)_{10}CH{=}CH_2$	182.35	1, 225	0.7658^{20}	1.4340^{20}	−13	232.8	79	s alc; v s eth
t266	Triethanolamine	$(HOCH_2CH_2)_3N$	149.19	4, 285	1.1242$^{20}_{4}$	1.4853^{20}	20.5	335.4	179	misc aq, alc, acet; 4.5 bz; 1.6 eth; s chl
t267	3,4,5-Triethoxybenzoic acid	$(C_2H_5O)_3C_6H_2CO_2H$	254.29	10, 481			110–112			
t268	Triethoxyborane	$(C_2H_5O)_3B$	145.99	1, 335	0.864	1.3740^{20}		117–118	11	dec aq
t269	Triethoxysilane	$(C_2H_5O)_3SiH$	164.28	1, 334	0.890	1.3770^{20}		134–135	26	
t270	3-(Triethoxysilyl)-propionitrile	$(C_2H_5O)_3SiCH_2CH_2CN$	217.34	4^{4}, 4271	0.979	1.4140^{20}		224	100	
t271	3-(Triethoxysilyl)-propyl isocyanate	$(C_2H_5O)_3Si(CH_2)_3NCO$	247.37		0.999	1.4200^{20}		283	77	
t272	Triethoxyvinylsilane	$(C_2H_5O)_3SiCH{=}CH_2$	190.32		0.903$^{20}_{4}$	1.3978^{20}		160–161	34	
t273	Triethylaluminum	$(C_2H_5)_3Al$	114.17	4, 643	0.832^{25}		−50	194	−18	dec aq, air
t274	Triethylamine	$(C_2H_5)_3N$	101.19	4, 99	0.7275^{20}	1.4010^{20}	−114.7	88.8	−7	5.5 aq; misc alc, eth; s acet, EtOAc
t275	Triethylantimony	$(C_2H_5)_3Sb$	208.94	4, 618	1.324^{16}	1.42	−29	159.5		
t276	Triethylarsine	$(C_2H_5)_3As$	162.11	4, 602	1.150$^{20}_{4}$			140^{736mm}		i aq; misc alc, eth
t277	Triethylborane	$(C_2H_5)_3B$	98.00	4, 641	0.6961^{23}	1.3970^{20}	−02.9	95		i aq; dec by air

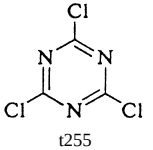
Trichloromethane, c145
(Trichloromethyl)benzene, t251
Tricyclophenylsilane, p159
3,3,3-Trichloropropylene oxide, e18

Tricine, t441
Tri-*o*-cresyl phosphate, t452
Tricyclene, t400a
Tricyclo[3.3.1.1^{3,7}]decane, a65

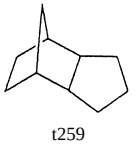
Tricyclo[5.2.1.0^{2,6}]decane-4,8-dimethanol, b202
3-Triethoxysilylpropylamine, a273
Triethyl borate, t268



t248



t255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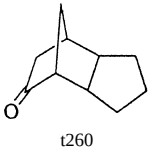


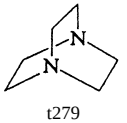
t260

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

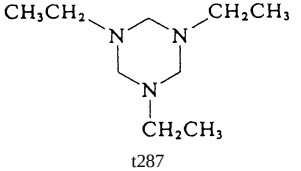
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
t278	Triethyl citrate	$HOC(CO_2C_2H_5)(CH_2CO_2C_2H_5)_2$	276.29	3, 568	1.137	1.4420^{20}		127^{1mm}	>110	
t279	Triethylenediamine		112.18	23^3, 484			158–160		62	45 aq; 13 acet; 77 alc; 51 bz
t280	Tri(ethylene glycol)	$(HOCH_2CH_2OCH_2\text{-})_2$	150.17	1, 468	1.1274^{15}	1.4550^{20}	−7	285	177	misc aq, alc, bz
t281	Tri(ethylene glycol) dimethacrylate	$[H_2C{=}C(CH_3)CO_2CH_2\text{-}CH_2OCH_2\text{-}]_2$	286.33	2^4, 1531	1.092	1.4605^{20}		172^{5mm}	>110	
t282	Tri(ethylene glycol) dimethyl ether	$(CH_3OCH_2CH_2OCH_2\text{-})_2$	178.23	Merck: 12, 9820	0.990^{20}_4	1.4224^{20}	−45	216	111	misc aq, hydrocarbon solvents
t283	Tri(ethylene glycol) divinyl ether	$H_2C{=}CH(OCH_2H_2)_3OCH{=}CH_2$	202.25	1^3, 2106	0.990	1.4530^{20}		126^{18mm}	>110	
t284	Tri(ethylene glycol) monomethyl ether	$CH_3(OCH_2CH_2)_3OH$	164.20	1^3, 2105	1.026	1.4399^{20}		122^{10mm}	>110	
t285	Triethylenetetramine	$(H_2NCH_2CH_2NHCH_2\text{-})_2$	146.24	4, 255	0.982	1.4971	12	266	143	
t286	Triethylgallium	$(C_2H_5)_3Ga$	156.91		1.0576^{30}		−82.3	142.6		
t287	1,3,5-Triethylhexahydro-1,3,5-triazine		171.20	26, 2	0.894	1.4595^{20}		207–208	80	
t288	Triethylindium	$(C_2H_5)_3In$	202.01		1.260^{20}	1.538^{20}	−32	144		
t289	Triethyl orthoacetate	$CH_3C(OC_2H_5)_3$	162.23	2, 129	0.8847^{25}_4	1.3950^{25}		142	36	misc alc, chl, eth
t290	Triethyl orthoformate	$HC(OC_2H_5)_3$	148.20	2, 20	0.891^{20}_4	1.3910^{20}	−76	146	30	dec aq; s alc, eth
t291	Triethyl orthopropionate	$CH_3CH_2C(OC_2H_5)_3$	176.26	2, 240	0.876	1.3995^{20}		155–160	60	v s alc, eth
t292	Triethyl phosphate	$(C_2H_5O)_3P(O)$	182.16	1, 332	1.0695^{20}	1.4058^{20}	−56	215	115	s aq(dec), alc, eth
t293	Triethylphosphine	$(C_2H_5)_3P$	118.16	4, 582	0.800^{15}_4	1.4563^{20}	−88	128–129	−17	i aq; misc alc, eth; pyrophoric
t294	Triethyl phosphite	$(C_2H_5O)_3P$	166.16	1, 330	0.969^{20}_4	1.4130^{20}		156	54	i aq(hyd); misc alc, acet, bz, eth, PE
t295	Triethyl phosphonoacetate	$(CH_3CH_2O)_2P(O)CH_2CO_2C_2H_5$	224.19	4^1, 573	1.130	1.4310^{20}		145^{9mm}	>110	
t296	Triethyl phosphonoformate	$(CH_3CH_2O)_2P(O)CO_2C_2H_5$	212.17	3^2, 103	1.110	1.4320^{20}		135^{12mm}	>110	
t297	Triethylsilane	$(C_2H_5)_3SiH$	116.28	4, 625	0.731^{20}_4	1.412^{20}		107–108	−3	i aq; misc alc, eth
t298	Triethyl thiophosphate	$(C_2H_5O)_3P(S)$	198.22	1, 333	1.082	1.4480^{20}		100^{16mm}	107	
t299	2,2,2-Trifluoroacetamide	CF_3CONH_2	113.04	2^2, 186			70–75	162.5		

t300	Trifluoroacetic acid	CF_3CO_2H	114.02	2^{2}, 186	1.4890^{20}	1.2850^{20}	−15.3	73		misc aq
t301	Trifluoroacetic anhydride	$[CF_3C(O)]_2O$	210.03	2^{2}, 186	1.487	<1.300	−65	39–40		
t302	1,1,1-Trifluoroacetone	$CF_3C(O)CH_3$	112.05	1^{2}, 717	1.252	<1.30		22	−30	
t303	1,3,5-Trifluorobenzene	$C_6H_3F_3$	132.09		1.277	1.4150^{20}	−5.5	75–76	−7	
t304	α,α,α-Trifluoro-*m*-cresol	$CF_3C_6H_4OH$	162.11	6^{1}, 187	1.333	1.4588^{20}	−1.8	178–179	73	
t305	2,2,2-Trifluoroethanol	CF_3CH_2OH	100.04	1^{3}, 1342	1.3842_4^{20}	1.2907^{20}	−43.5	74	29	
t306	2,2,2-Trifluoroethyl trifluoroacetate	$CF_3CH_2O_2CCF_3$	196.05	2^{3}, 427	1.4725_4^{18}	1.2812^{18}	−65.5	55	0	
t307	Trifluoromethane	HCF_3	70.01	1, 59	1.52^{-100}		−160	−84		75 mL aq; 500 mL alc
t308	Trifluoromethanesulfonic acid	CF_3SO_3H	150.07	3^{4}, 34	1.695^{25}	1.3250^{25}	34	162	none	v s aq; misc eth
t309	Trifluoromethanesulfonic anhydride	$(CF_3SO_2)_2O$	282.13	3^{4}, 35	1.677	1.3212^{20}		84	none	dec aq, alc
t310	3-(Trifluoromethyl)aniline	$CF_3C_6H_4NH_2$	161.13	12, 870	1.290	1.4800^{20}	5–6	187	85	
t311	α,α,α-Trifluorotoluene	$C_6H_5CF_3$	146.11	5, 290	1.1886^{20}	1.4145^{20}	−29	102	12	
t312	Trihexyl *O*-acetylcitrate	$CH_3CO_2C[CO_2(CH_2)_5CH_3]$-$[CH_2CO_2(CH_2)_5CH_3]_2$	486.65		1.005	1.4470^{20}			>110	
t313	Trihexylamine	$[CH_3(CH_2)_5]_3N$	269.52	4, 188	0.794	1.4415^{20}		163–265	>110	v s alc, eth; i aq
t314	Trihexyl *O*-butylcitrate	$C_3H_7CO_2C[CO_2(CH_2)_5CH_3]$-$[CH_2CO_2(CH_2)_5CH_3]_2$	514.71		0.993	1.4480^{20}	−55		>110	
t315	Trihexylchlorosilane	$[CH_3(CH_2)_5]_3SiCl$	319.12		0.871_4^{20}	1.456^{20}		155^{5mm}		

Triethylenediamine, d61
Triethylene glycol, e139
Triethylene glycol dimethyl ether, b211
O,*O*,*O*-Triethyl phosphorothioate, t298
2,2,2-Trifluoroethyl mesylate, m453
2-(Trifluoromethyl)aniline, a126
3-(Trifluoromethyl)aniline, a127
Trifluoromethylbenzene, t311
m-Trifluoromethylphenol, t304
4,4,4-Trifluoro-1-(2-thienyl)-1,3-butanedione, t132
α,α,α-Trifluorotoluidines, a126 thru a128
Triglyme, b211



t279



t287

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
t316	Trihexylsilane	$[CH_3(CH_2)_5]_3SiH$	284.60	4^4, 3915	0.799	1.448^{20}		161	>110	
t317	1,2,3-Trihydroxybenzene	$C_6H_3(OH)_3$	126.11	6, 1071	1.45		133	309		59 aq; 77 alc; 62 eth
t318	1,3,5-Trihydroxybenzene	$C_6H_3(OH)_3$	126.11	6, 1092			218–221			1 aq; 10 alc; s eth
t319	3,4,5-Trihydroxybenzoic acid	$(HO)_3C_6H_2CO_2H$	170.12	10, 470			258–265			1.1 aq; 17 alc; 1 eth; 20 acet; i bz, chl, PE
t320	2,3,4-Trihydroxybenzophenone	$(HO)_3C_6H_2COC_6H_5$	230.22	8, 417			140–142			
t321	1,2,6-Trihydroxyhexane	$HO(CH_2)_4CH(OH)CH_2OH$	134.18	1,*4*, 2784	1.109	1.4760^{20}		178^{5mm}	79	
t322	Triisobutylaluminum	$[(CH_3)_2CHCH_2]_3Al$	198.33	4, 643	0.786	1.4494^{20}	4–6	86^{10mm}	−18	pyrophoric
t323	Triisobutylamine	$[(CH_3)_2CHCH_2]_3N$	185.36	4, 166	0.766	1.4230^{20}		192–193	57	
t324	Triisodecyl phosphite	$[(CH_3)_2CH(CH_2)_7O]_3P$	502.80		0.884	1.4600^{20}	<0	166	235	
t325	Triisopropanolamine	$[CH_3CH(OH)CH_2]_3N$	191.27	4^3, 762	0.9996^{50}_{20}		48–52	305.4	152	v s aq
t326	Triisopropoxyborane	$[(CH_3)_2CHO]_3B$	188.08	1, 363	0.815	1.3764^{20}		139–141	10	
t327	1,3,5-Triisopropylbenzene	$C_6H_3[CH(CH_3)_2]_3$	204.36	5, 458	0.845	1.4880^{20}		232–236	86	
t328	Triisopropyl orthoformate	$CH[OCH(CH_3)_2]_3$	190.29	2^3, 39	0.854	1.3970^{20}		66^{18mm}	42	
t329	Triisopropyl phosphite	$[(CH_3)_2CHO]_3P$	208.24	1, 363	0.914^{20}_4	1.4110^{20}		64^{11mm}	67	i aq(sl hyd)
t330	Triisopropylsilane	$[(CH_3)_2CH]_3SiH$	158.36	4^3, 1851	0.773	1.4344^{20}		86^{35mm}	37	
t331	3,4,5-Trimethoxybenzaldehyde	$(CH_3O)_3C_6H_2CHO$	196.20	8, 391			73–75	165^{10mm}		
t332	1,2,3-Trimethoxybenzene	$C_6H_3(OCH_3)_3$	168.19	6, 1081	1.112		43–45	241	>110	
t333	1,2,4-Trimethoxybenzene	$C_6H_3(OCH_3)_3$	168.19	6, 1088	1.126	1.5330^{20}		247	>110	
t334	1,3,5-Trimethoxybenzene	$C_6H_3(OCH_3)_3$	168.19	6, 1101			51–53	255	85	
t335	3,4,5-Trimethoxybenzoic acid	$(CH_3O)_3C_6H_2CO_2H$	212.20	10, 481			168–171	227^{10mm}		v s alc, eth; s chl

t336	3,4,5-Trimethoxybenzoyl chloride	$(CH_3O)_3C_6H_2COCl$	230.65	10, 487			81–84	185^{18mm}		
t337	3,4,5-Trimethoxybenzyl alcohol	$(CH_3O)_3C_6H_2CH_2OH$	198.22	6, 1159	1.233	1.5439^{20}		228^{25mm}	>110	
t338	Trimethoxyborane	$(CH_3O)_3B$	103.91	1, 287	0.920^{23}_{4}	1.3568^{20}	−34	67–68	−13	hyd aq; misc alc, eth
t339	Trimethoxyboroxine	$[-OB(OCH_3)-]_3$	173.53		1.195	1.3996^{20}	10	130	10	
t340	1,1,2-Trimethoxyethane	$CH_3OCH_2CH(OCH_3)_2$	120.15	1[3], 3183	0.932	1.3921^{20}		59^{56mm}	23	
t341	1,1,3-Trimethoxypropane	$CH_3OCH_2CH_2CH(OCH_3)_2$	134.18	1, 820	0.942	1.4004^{20}		46^{17mm}	40	
t342	1,1,3-Trimethoxypropylsilane	$CH_3OCH_2CH_2CH_2Si(OCH_3)_3$	164.28		0.932	1.3900^{20}		142	40	
t343	Trimethoxysilane	$(CH_3O)_3SiH$	122.20	1[2], 274	0.960	1.3579^{20}	−115	81	−4	
t344	3-(Trimethoxysilyl)propylamine	$H_2N(CH_2)_3Si(OCH_3)_3$	179.29		1.027	1.4240^{20}		92^{15mm}	83	
t345	*N*-[3-(Trimethylsilyl)propyl]aniline	$C_6H_5NH(CH_2)_3Si(OCH_3)_3$	255.39		1.070	1.5550^{20}		310	>110	
t346	*N*[1]-[3-(Trimethoxysilyl)propyl]ethylenediamine	$(CH_3O)_3Si(CH_2)_3NHCH_2CH_2NH_2$	224.36		1.019	1.4450^{20}		146^{15mm}	>110	
t347	3-(Trimethoxysilyl)propyl methacrylate	$(CH_3O)_3Si(CH_2)_3O_2CC(CH_3)=CH_2$	248.35		1.045^{20}_{4}	1.4310^{20}		190	92	
t348	[3-(Trimethoxysilyl)propyl]urea	$(CH_3O)_3Si(CH_2)_3NHCONH_2$	222.32		1.150	1.4600^{20}		217–250	98	
t349	Trimethylacetic acid	$(CH_3)_3CCO_2H$	102.13	2, 319	0.889		33–35	163–164	63	
t350	Trimethylacetic anhydride	$[(CH_3)_3CCO]_2O$	186.25	2, 320	0.918	1.4090^{20}		193	57	
t351	Trimethylacetyl chloride	$(CH_3)_3CCOCl$	120.58	2, 320	0.979	1.4120^{20}		105–106	8	
t352	Trimethylaluminum	$(CH_3)_3Al$	72.09	4, 643	0.752^{20}	1.432^{12}	15	125–126	−18	s alk; v sl s alc

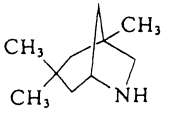
Tri-(2-hydroxyethyl)amine, t266
1,2,6-Trihydroxyhexane, h63
1,2,3-Trihydroxypropane, g19
Triiodomethane, i33
Trimellitic acid, b30
Trimellitic anhydride, b32
Trimesic acid, b31
Trimesoyl chloride, b33
Trimethoxymethylsilane, m455
Trimethylacetaldehyde, d677
Trimethylacetamide, d678
Trimethylacetic acid, d679
Trimethylacetic anhydride, d680
Trimethylacetyl chloride, d681

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
t354	Trimethylamine	$(CH_3)_3N$	59.11	4, 43	0.656	1.3631^{0}	−117	2.9	−7	41 aq; misc alc; s bz, chl, eth
t355	2,4,6-Trimethylaniline	$(CH_3)_3C_6H_2NH_2$	135.21	12, 1160	0.963	1.5510^{20}		233	96	
t356	1,3,3-Trimethyl-6-aza-bicyclo[3.2.1]octane		153.27		0.902	1.4716^{20}		194	75	
t357	1,2,3-Trimethyl-benzene	$C_6H_3(CH_3)_3$	120.20	5, 399	0.8944_4^{20}	1.5139^{20}	−25.4	176.1	48	i aq; s alc, eth
t358	1,2,4-Trimethyl-benzene	$C_6H_3(CH_3)_3$	120.20	5, 400	0.8756_4^{20}	1.5048^{20}	−43.9	169	48	s alc, bz, eth
t359	1,3,5-Trimethyl-benzene	$C_6H_3(CH_3)_3$	120.20	5, 406	0.8637_4^{20}	1.4994^{20}	−44.7	165	44	misc alc, bz, eth
t360	Trimethyl 1,2,4-benzenetri-carbox-ylate	$C_6H_3(CO_2CH_3)_3$	252.22	9[1], 429	1.261	1.5214^{20}	38–40	194^{12mm}	>110	
t361	2,2,3-Trimethylbutane	$(CH_3)_2CHC(CH_3)_3$	100.20	1[2], 121	0.6901_4^{20}	1.3890^{20}	−24.9	80.9	−6	s alc, eth
t362	2,3,3-Trimethyl-2-butanol	$(CH_3)_3CC(CH_3)_2OH$	116.20	1[2], 447	0.8380_4^{25}	1.4233^{22}	15–17	130.5		misc alc, eth
t363	1,2,4-Trimethylcyclo-hexane	$C_6H_9(CH_3)_3$	126.24	5, 42	0.786	1.4330^{20}		141–143	18	
t364	3,5,5-Trimethylcyclo-hex-2-ene-1-one		138.2	7, 65	0.918	1.4720^{20}	−8.1	215	80	1.2 aq
t365	2,6,6-Trimethyl-2-cyclohexene-1,4-dione		152.19	7[4], 2032		1.4910^{20}	26–28	94^{11mm}	96	
t366	Trimethyl-1,6-diiso-cyanatohexane	$OCNCH_2CH_2C(CH_3)CH_2$-$C(CH_3)CH_2CNO$	210.28		1.012	1.4620^{20}		149	>110	
t367	2,2,6-Trimethyl-4*H*-1,3-dioxin-4-one		142.16	19[3], 1604	1.088	1.4620^{20}	12–13	67^{2mm}	86	
t368	4,4′-Trimethylenebis-(1-methylpiperidine)		238.42		0.896	1.4820^{20}	13	215^{50mm}	>110	
t369	4,4′-Trimethylene-dipiperidine		210.37				65–58			
t370	3,5,5-Trimethylhexanal	$(CH_3)_3CCH_2CH(CH_3)CH_2CHO$	142.24	1[3], 2894	0.817	1.4215^{20}		$68^{2.4mm}$	46	

t370a	3,5,5-Trimethylhexane	$(CH_3)_2CHCH_2CH(CH_3)CH(CH_3)_2$	128.26		0.7218^{20}	1.4051^{20}	−128	131		
t371	3,5,5-Trimethyl-1-hexanol	$(CH_3)_3CCH_2CH(CH_3)$-CH_2CH_2OH	144.25	1^3, 1755	0.8236^{20}_4	1.4300^{25}	< −70	193–194	80	s alc, eth
t372	3,5,5-Trimethyl-hexanoyl chloride	$(CH_3)_3CCH_2CH(CH_3)$-CH_2COCl	176.89	2^3, 834	0.930	1.4360^{20}		188–190	140	
t374	Trimethylhydro-quinone	$(CH_3)_3C_6H(OH)_2$	152.19	6, 931			172–174			s aq; v s alc, bz, eth
t375	1,3,3-Trimethyl-2-norbornanol		154.25	6, 70	0.9641^{20}_4		39–45	201	73	s alc, eth

endo-1,7,7-Trimethylbicyclo[2.2.1]heptan-2-ol, b245
2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene, p175
1,7,7-Trimethylbicyclo[2.2.1]hepten-2-one, c3
Trimethyl borate, t338
Trimethylchlorosilane, c266
α,α,4-Trimethyl-3-cyclohexene-1-methanol, t13
3,5,5-Trimethylcyclohex-2-en-1-one, i93
1,2,2-Trimethyl-1,3-cyclopentanedicarboxylic acid, c4
Trimethylene chlorobromine, b307
Trimethylene chlorohydrin, c231
Trimethylenediamine, p190
Trimethylene dibromide, d121
Trimethylene dimercaptan, p195
Trimethylene glycol, p192
Trimethylethylene, m166
Trimethylgermanium bromide, b437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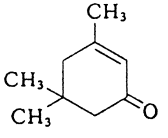
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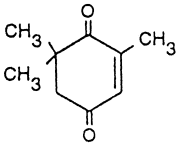
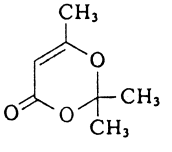

t365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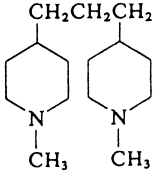
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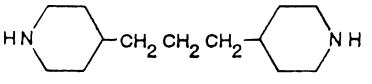
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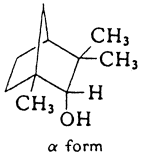
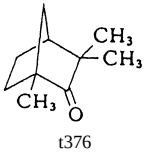

α form
t375

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
t376	1,3,3-Trimethyl-2-norbornanone		152.24	7, 96	0.948^{18}	1.4635^{18}	5	192–194	52	v s alc, eth
t377	Trimethyl orthoacetate	$CH_3C(OCH_3)_3$	120.15	2^2, 128	0.9428^{25}_{4}	1.3859^{25}		107–109	16	v s alc, eth
t378	Trimethyl orthoformate	$HC(OCH_3)_3$	106.12	2, 19	0.9676^{20}_{4}	1.3790^{20}		100.6	15	
t379	2,4,4-Trimethyl-2-oxazoline		113.16		0.887	1.4213^{20}		112–113	12	
t380	2,2,3-Trimethylpentane	$(CH_3)_3CCH(CH_3)CH_2CH_3$	114.23	1^1, 62	0.7160^{20}_{4}	1.4030^{20}	−112.3	110	<21	s eth; sl s alc
t381	2,2,4-Trimethylpentane	$(CH_3)_2CHCH_2C(CH_3)_3$	114.23	1^2, 127	0.6919^{20}_{4}	1.3915^{20}	−107.4	99.2	−12	s bz, chl, eth
t382	2,3,4-Trimethylpentane	$(CH_3)_2CH[CH(CH_3)]_2CHCH_3$	114.23	1^3, 500	0.7190^{20}_{4}	1.4042^{20}	−109.2	113–114	5	s alc, org solv
t383	2,2,4-Trimethyl-1,3-pentanediol	$(CH_3)_2CHCH(OH)C(CH_3)_2CH_2OH$	146.22	1^3, 2225	0.928^{55}_{15}	1.4513^{15}	52–56	232	113	1.8 aq; 75 alc; 22 bz; 25 acet
t384	2,4,4-Trimethyl-1-pentene	$(CH_3)_3CCH_2C(CH_3)=CH_2$	112.22	1^3, 849	0.7150^{20}_{4}	1.4112^{20}	−93	101–102	−6	
t385	2,3,5-Trimethylphenol	$(CH_3)_3C_6H_2OH$	136.19	6, 518			92–95	230–231		
t386	2,3,6-Trimethylphenol	$(CH_3)_3C_6H_2OH$	136.19				62–64			
t387	2,4,6-Trimethylphenol	$(CH_3)_3C_6H_2OH$	136.19	6, 518			71–74	220		
t388	2,4,6-Trimethyl-1,3-phenylenediamine	$(CH_3)_3C_6H(NH_2)_2$	152.23	13^1, 190			88–91			
t389	Trimethyl phosphate	$(CH_3O)_3P(O)$	140.08	1, 286	1.197^{20}	1.3967^{20}	−46	197	107	100 aq; s alc
t390	Trimethyl phosphite	$(CH_3O)_3P$	124.08	1, 285	1.046^{20}_{4}	1.4080^{20}	−78	111–112	27	dec aq; misc alc, acet, bz, PE
t391	Trimethyl phosphonoacetate	$(CH_3O)_2P(O)CH_2CO_2CH_3$	182.11		1.125	1.4370^{20}		$118^{0.85mm}$	>110	
t392	1,2,4-Trimethylpiperazine		128.22		0.851^{25}_{25}	1.4480^{25}	−50	151^{746mm}		s aq, alc, acet, bz
t393	2,4,6-Trimethylpyridine	$C_5H_2N(CH_3)_3$	121.18	20, 250	0.9166^{22}_{4}	1.4959^{25}	−46	171	57	3.5 aq; misc eth; s alc, bz, chl
t394	*N*-(Trimethylsilyl)-acetamide	$CH_3CONHSi(CH_3)_3$	131.25				46–49	186	57	
t395	Trimethylsilyl acetate	$CH_3CO_2Si(CH_3)_3$	132.24	4^3, 1857	0.882	1.3880^{20}	−32	108	4	
t396	*N*-(Trimethylsilyl)-imidazole		140.26		0.956	1.4751^{20}		94^{14mm}	5	

t397	Trimethylsilyl methacrylate	$H_2C{=}C(CH_3)CO_2Si(CH_3)_3$	158.28		0.890	1.4150^{20}		51^{20mm}	32	
t398	Trimethylsilyl trifluoromethane sulfonate	$CF_3SO_3Si(CH_3)_3$	222.26		1.228	1.3600^{20}		77^{80mm}	25	
t399	Trimethylsulfonium iodide	$[(CH_3)_3S]I$	204.07					215–220 sublime		
t400	Trimethylsulfoxonium iodide	$[(CH_3)_3S(O)]I$	220.07				169 dec			
t400a	1,7,7-Trimethyltricyclo[2.2.1.$O^{2,6}$]-heptane		136.24	5, 164	0.8668^{80}	1.4296^{80}	67.5	152.5		
t401	Trimethylvinylsilane	$(CH_3)_3SiCH{=}CH_2$	100.24		0.649	1.3920^{20}		55	< -34	
t402	2,4,6-Trinitroaniline	$(O_2N)_3C_6H_2NH_2$	228.12	12, 763	1.762^{14}		188–190	explodes		s hot acet; sl s alc
t403	1,2,4-Trinitrobenzene	$C_6H_3(NO_2)_3$	213.11	5, 271	1.73^{16}		61–62	explodes		5.5 alc; 7.1 eth; i aq
t404	1,3,5-Trinitrobenzene	$C_6H_3(NO_2)_3$	213.11	5, 271	1.688_4^{20}		122.5	explodes		0.035 aq; 1.9 alc; 1.5 eth; 6.2 bz
t405	2,4,6-Trinitrotoluene	$(O_2N)_3C_6H_2CH_3$	227.13	5, 347	1.654_4^{20}		80.1	explodes		1.5 alc; 4 eth; s bz, acet; 0.01 aq
t406	Trioctylamine	$[(CH_3(CH_2)_7]_3N$	353.68	4, 196	0.809	1.4485^{20}		365–367	>110	
t407	1,3,5-Trioxane		90.08	19, 381	1.170^{65}		60.2	115	45	17.2 aq[18]; v s alc, bz, eth, EtOAc

Trimethylolpropane, e183
Trimethylolpropane triacrylate, e114
Trimethylolpropane trimethacrylate, e185
1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane, c277
Trimethylsilyl cyanide, c331
(*N*-Trimethyl)silyldiethylamine, d404
(*N*-Trimethyl)silyldimethylamine, d726
Trimethylsilyl iodide, i56
Trimethylsilylnitrile, c331
2,4,6-Trinitrophenol, p174
Triolein, g23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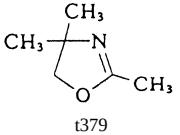
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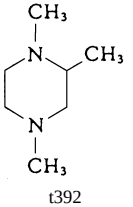
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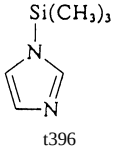
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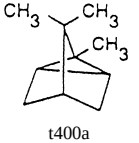

t400a

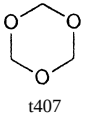

t407

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
t408	4,7,10-Trioxa-1,13-tridecanediamine	$O[CH_2CH_2O(CH_2)_3NH_2]_2$	220.31	4,*4*, 1625	1.005	1.4640^{20}		148^{4mm}	>110	
t409	Tripentaerythritol	$(HOCH_2)_3CCH_2OCH_2$-$C(CH_2OH)_2CH_2OCH_2$-$C(CH_2OH)_3$	372.41				225 dec			
t410	Triphenylamine	$(C_6H_5)_3N$	245.33	12, 181	0.774_0^0		125–127	347–348		
t411	Triphenylantimony	$(C_6H_5)_3Sb$	353.07	16, 891	1.4343^{25}		52–54	377	>110	v s bz, eth; sl s alc
t412	Triphenylarsine	$(C_6H_5)_3As$	306.24	16, 828	1.2225^{48}	1.6139^{48}	60–62	233^{14mm}		v s bz, eth; s alc
t413	1,3,5-Triphenylbenzene	$(C_6H_5)_3C_6H_3$	306.41	5, 737	1.205		172–174	460		v s bz; s abs alc, eth
t414	Triphenylborane	$(C_6H_5)_3B$	242.13	16^2, 636			145	203^{15mm}		
t415	Triphenylmethane	$(C_6H_5)_3CH$	244.34	5, 698	1.0134_4^{99}		92–94	360		v s hot alc, eth; 49 chl; 7 bz; s PE
t416	Triphenylmethanol	$(C_6H_5)_3COH$	260.34	6, 713	1.199_4^0		160–163	360		v s alc, bz, eth; i aq
t417	Triphenylmethyl bromide	$(C_6H_5)_3CBr$	323.24	5, 704			152–154	230^{15mm}		
t418	Triphenylmethyl chloride	$(C_6H_5)_3CCl$	278.78	5, 700			110–112	235^{20mm}		
t419	Triphenyl phosphate	$(C_6H_5O)_3P(O)$	326.29	6, 179			50–52	244^{10mm}	223	misc alc; s bz, acet, chl, eth; i aq
t420	Triphenylphosphine	$(C_6H_5)_3P$	262.29	16, 759	1.075_4^{81}		79–81	377	181	v s eth; s bz, chl, HOAc; sl s alc; i aq
t421	Triphenylphosphine oxide	$(C_6H_5)_3P(O)$	278.29	16, 783			156–158			
t422	Triphenyl phosphite	$(C_6H_5O)_3P$	310.29	6, 177	1.184	1.5903^{20}	22–24	360	218	s alc, bz, chl, eth
t423	Triphenylsilane	$(C_6H_5)_3SiH$	260.41	16^2, 605			42–44	152^{2mm}	76	
t424	Triphenyltin acetate	$CH_3CO_2Sn(C_6H_5)_3$	409.06	16^4, 1606			124–126			s eth; sl s alc, bz
t425	Triphenyltin chloride	$(C_6H_5)_3SnCl$	385.46	16, 914			108 dec	$240^{13.5mm}$		
t426	Triphenyltin hydroxide	$(C_6H_5)_3SnOH$	367.02	16, 914			124–126			
t427	Tripropoxyborane	$(CH_3CH_2CH_2O)_3B$	188.08	1^2, 369	0.8576_4^{20}	1.3948^{20}		175–177	32	v s alc; misc eth
t428	Tripropylaluminum	$(CH_3CH_2CH_2)_3Al$	156.25	4, 643	0.823		−107	84^{2mm}	−18	
t429	Tripropylamine	$(CH_3CH_2CH_2)_3N$	143.27	4, 139	0.753	1.4160^{20}	−93.5	155–158	36	s aq, alc, eth
t430	Tripropylene glycol	$H(OCH_2CH_2CH_2)_3OH$	192.26		1.021	1.442^{25}		273	141	s aq

t431	Tripropylene glycol butyl ether	$HO(CH_2CH_2CH_2O)_3(CH_2)_3CH_3$	248.4		0.932	1.430^{20}		276	135	
t432	Tripropylene glycol monomethyl ether	$HO(CH_2CH_2CH_2O)_3CH_3$	206.29	1[4], 2475	0.967	1.428^{25}	−42	242.4	127	misc aq, alc, eth
t433	Tripropyl orthoformate	$HC(OCH_2CH_2CH_3)_3$	190.28	2, 21	0.8805_4^{20}	1.4072^{20}		108^{40mm}	72	
t434	Tris(2-aminoethyl)-amine	$(H_2NCH_2CH_2)_3N$	146.24	4, 256	0.977	1.4970^{20}		114^{15mm}	>110	
t435	Tris(2-butoxyethyl) phosphate	$(C_4H_9OCH_2CH_2O)_3P(O)$	398.48		1.006	1.4359^{20}		228^{4mm}	110	
t436	Tris(2-chloroethyl) phosphate	$(ClCH_2CH_2O)_3P(O)$	285.49	1[2], 337	1.390	1.4721^{20}		330	232	
t437	Tris(2-chloroethyl) phosphite	$(ClCH_2CH_2O)_3P$	269.49		1.353_4^{20}	1.4863^{20}		115^{2mm}	190	misc alc, bz, eth
t438	Tris(2-ethylhexyl) phosphate	$[C_4H_9CH(C_2H_5)CH_2O]_3P(O)$	434.65	1[3], 1734	0.924	1.4437^{20}		215^{4mm}	>110	i aq
t439	Tris(hydroxymethyl)-aminomethane	$(HOCH_2)_3CNH_2$	121.14	4, 303			171–172	220^{10mm}		
t440	1,1,1-Tris(hydroxy-methyl)ethane	$CH_3C(CH_2OH)_3$	120.15	1, 520			200–203			
t441	*N*-[Tris(hydroxy-methyl)methyl]-glycine	$(HOCH_2)_3CNHCH_2CO_2H$	179.17	Merck: 12, 9783			187			satd aq[0] is 0.8*M*
t442	Tris(hydroxymethyl)-nitromethane	$(HOCH_2)_3CNO_2$	151.12	1, 520			214 pure 175 tech			220 aq; v s alc; sl s bz
t443	Tris[2-(2-methoxy-ethoxy)ethyl]amine	$(CH_3OCH_2CH_2OCH_2CH_2)_3N$	323.43		1.011	1.4486^{20}			>110	
t444	Tris(2-methoxy-ethoxy)-vinylsilane	$H_2C{=}CHSi(OCH_2CH_2{-}OCH_3)_3$	280.39	4[4], 4257	1.034_4^{25}	1.427^{25}		284–286	>110	
t445	Tris(2-methoxyethyl) borate	$(CH_3OCH_2CH_2O)_3B$	236.08	1[3], 2118	1.010	1.4150^{20}		135^{15mm}	87	
t446	Tris(2-methylallyl)-amine	$[H_2C{=}C(CH_3)CH_2]_3N$	179.31	4[3], 462	0.794	1.4575^{20}		85^{15mm}	53	

Trioxymethylene, t407
Tripalmitin, g24
Triphenylmethyl bromide, b440
Triphenyl azide, a310
Triphenyltin chloride, c267
Tripropyl borate, t427
TRIS, t439
Tris(dimethylamino)phosphine oxide, h50
Tris(dimethylamino)silyl chloride, c268a
Tris(3,5-dioxaheptyl)amine, t443
Tris(7-methylnonyl) phosphite, t324
Tris(2-methylphenyl) phosphate, t452

TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

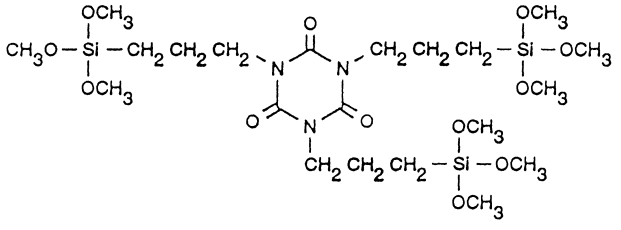
No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
t447	Tris(2,2,2-trifluoro-ethyl) phosphite	$(CF_3CH_2O)_3P$	328.07	1^4, 1371	1.487	1.3245^{20}		131^{743mm}	>110	
t448	Tris[3-(trimethoxy-silyl)propyl] isocyanurate		615.86		1.170	1.4610^{20}		250	102	
t449	Tris(trimethylsilyl) borate	$[(CH_3)_3SiO]_3B$	278.38	4^3, 1861	0.831	1.3861^{20}		186	42	
t450	1,3,5-Trithiane		138.27	19, 382			216–218			s bz; sl s alc, eth
t451	Trithiocarbonic acid	$(HS)_2CS$	110.21	3, 221	1.483_4^{20}	1.8225^{20}	−26.9	57.8		dec aq, alc; sl s eth
t452	Tri-*o*-tolyl phosphate	$(CH_3C_6H_4O)_3P(O)$	368.37	Merck: 12, 9893	1.1955^{20}	1.5575^{20}	11	410	225	sl s aq, alc; s eth
t453	1,2,4-Trivinylcyclo-hexane	$(H_2C{=}CH)_3C_6H_9$	162.28		0.836	1.4780^{20}		88^{20mm}	68	
t454	L-(−)-Tryptophan		204.23	22, 546			280–285 dec			1.14 aq[25]; s hot alc, alk; i eth, chl
t455	L-Tyrosine	$(HO)C_6H_4CH_2CH(NH_2)CO_2H$	181.19	14, 605	1.456		342–344			0.045 aq; 0.01 alc; s alk; i eth
u1	Undecanal	$CH_3(CH_2)_9CHO$	170.30	1, 712	0.825	1.4322^{20}	−4	115^{5mm}	96	i aq; s alc, eth
u2	Undecane	$CH_3(CH_2)_9CH_3$	156.31	1, 170	0.7402_4^{20}	1.4173^{20}	−25.6	196	60	i aq; misc alc, eth
u3	Undecanenitrile	$CH_3(CH_2)_9CN$	167.30	2, 358	0.823	1.4330^{20}		253	>110	
u4	Undecanoic acid	$CH_3(CH_2)_9CO_2H$	186.30	2, 358	0.8907	1.4294^{45}	28.5	228^{160mm}	>110	s alc, chl, eth; i aq
u5	Undecanoic γ-lactone		184.28	17, 247	0.949	1.4500^{20}		166^{13mm}	>110	
u6	Undecanoic δ-lactone		184.28	17^3, 4257	0.969	1.4590^{20}		$155^{10.5mm}$	>110	
u7	1-Undecanol	$CH_3(CH_2)_{10}OH$	172.31	1, 427	0.8324	1.4402^{20}	11	242.8	>110	
u8	2-Undecanol	$CH_3(CH_2)_8CH(OH)CH_3$	172.31	1, 427	0.828	1.4370^{20}	2–3	131^{28mm}	88	
u9	2-Undecanone	$CH_3(CH_2)_8COCH_3$	170.30	1, 173	0.829	1.4300^{20}	11–13	231–232	88 (CC)	s alc, bz, chl, eth, acet; i aq
u10	3-Undecanone	$CH_3(CH_2)_7COCH_2CH_3$	170.30	1, 713	0.827	1.4291^{20}	12–13	225–229	89	
u11	6-Undecanone	$CH_3(CH_2)_4CO(CH_2)_4CH_3$	170.30	1, 174	0.831	1.4280^{20}	14.6	228	88	i aq; v s alc, eth
u12	10-Undecenal	$H_2C{=}CH(CH_2)_8CHO$	168.28	1,*3*, 3029	0.810	1.4427^{20}			92	
u12a	1-Undecene	$H_2C{=}CH(CH_2)_8CH_3$	154.30	1, 225	0.7503^{20}	1.4261^{20}	−49	193	71	
u13	10-Undecenoic acid	$H_2C{=}CH(CH_2)_8CO_2H$	184.28	2, 458	0.907_4^{24}	1.4493^{20}	24.5	137^{2mm}	148	s alc, chl, eth; i aq
u14	10-Undecen-1-ol	$H_2C{=}CH(CH_2)_9OH$	170.30	1, 452	0.850^{15}	1.4500^{20}	−2	245	93	

u15	10-Undecenoyl chloride	$H_2C{=}CH(CH_2)_8COCl$	202.73	2, 459	0.944	1.4540^{20}		122^{10mm}	93	
u16	Urea	$(H_2N)_2CO$	60.06	3, 42	1.335		133–135	dec > mp		100 aq; 20 alc
u17	Uric acid		168.11	26, 513	1.893^{20}		>300 dec			s alk; i aq, alc, eth
u18	Uridine		244.20	31, 23			166–167			s aq; hot alc, pyr

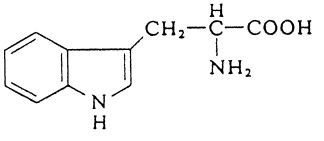
Trityl alcohol, t416
Triptamine, a170
Tyramine, a173
Umbelliferone, h111

Undecyl alcohol, u7
Undecylenic aldehyde, u12
Undecyl-10-en-1-oic acid, u13
Undecylic aldehyde, u1

Undecyl iodide, i57
Uracil, p278
4-Ureidohydantoin, a71
Urethane, e102


t448


t450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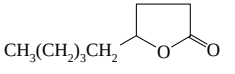
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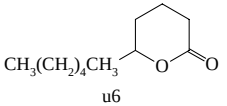
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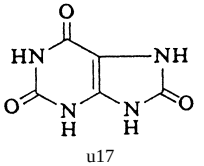
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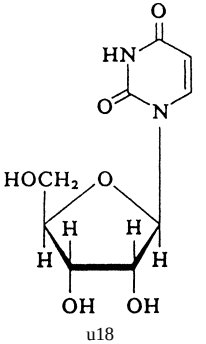

u18

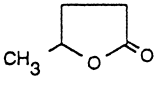
TABLE 1.15 Physical Constants of Organic Compounds (*Continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density, g/mL	Refractive index	Melting point,°C	Boiling point,°C	Flash point,°C	Solubility in 100 parts solvent
v1	Valeric anhydride	$[CH_3(CH_2)_3CO]_2O$	186.25	2, 301	0.942	1.4210^{20}	−57	112^{16mm}	101	
v2	γ-Valerolactone		100.12	17, 235	1.057	1.4330^{20}	−31	207–208	81	
v3	δ-Valerolactone		100.12	17, 235	1.079	1.4580^{20}		$60^{0.5mm}$	100	
v4	L-Valine	$(CH_3)_2CHCH(NH)CO_2H$	117.15	4, 427	1.230		>315 subl			8.8 aq; v sl s alc, eth
v5	Vinyl acetate	$H_2C{=}CHO_2CCH_3$	86.09	2^1, 63	0.932_4^{20}	1.3954^{20}	−93	72–73	−8	2 aq; misc alc, eth
v6	Vinyl benzoate	$C_6H_5CO_2CH{=}CH_2$	148.16	9^1, 65	1.070	1.5290^{20}		96^{20mm}	82	
v7	4-Vinylbenzyl chloride	$H_2C{=}CHC_6H_4CH_2Cl$	152.62		1.083	1.5740^{20}		229	104	
v8	Vinylcyclohexane	$C_6H_{11}CH{=}CH_2$	110.20	5^1, 35	0.805	1.4463^{20}		126–127	20	
v9	4-Vinyl-1-cyclohexene		108.18	5^1, 63	0.803_4^{20}	1.4640^{20}	−101	127	20	
v10	2-Vinyl-1,3-dioxolane		100.12		1.001	1.4300^{20}		115–116	14	
v11	*N*-Vinylformamide	$HCONHCH{=}CH_2$	71.08		1.014	1.4940^{20}	−16	210	102	
v12	1-Vinylimidazole		94.12	23^4, 569	1.039	1.5308^{20}		79^{13mm}	81	
v13	5-Vinyl-2-norbornene		120.20		0.841	1.4802^{20}	−80	141	27	
v14	Vinyl propionate	$CH_3CH_2CO_2CH{=}CH_2$	100.12	2^3, 532	0.919	1.4030^{20}	−80	94–95	6	
v15	2-Vinylpyridine	$(C_5H_4N)CH{=}CH_2$	105.14	20, 256	0.975	1.5490^{20}		158–159	46	v s alc, chl, eth
v16	4-Vinylpyridine	$(C_5H_4N)CH{=}CH_2$	105.14	20^2, 170	0.975	1.5500^{20}		65^{15mm}	51	sl s hot aq, hot alc
v17	*N*-Vinyl-2-pyrrolidinone		111.14		1.040	1.5120^{20}		93^{13mm}	93	
v18	Vinyltrimethoxysilane	$H_2C{=}CHSi(OCH_3)_3$	148.24		0.968	1.3920^{20}		123	22	
x1	Xanthene		182.22	17, 73			101	310–312		s bz, eth; sl s alc, aq
x2	Xanthen-9-carboxylic acid		226.23	18^2, 279			217 dec			s hot alc, eth
x3	9-Xanthenone		196.21	17, 354			174–176	350^{730mm}		0.5 alc; v s chl
x4	*m*-Xylene	$C_6H_4(CH_3)_2$	106.17	5, 370	0.8642^{20}	1.4972^{20}	−47.9	139	27	misc alc, eth; 0.02 aq
x5	*o*-Xylene	$C_6H_4(CH_3)_2$	106.17	5, 362	0.8808_4^{20}	1.5054^{20}	−25.2	144–145	32	misc alc, eth; 0.017 aq
x6	*p*-Xylene	$C_6H_4(CH_3)_2$	106.17	5, 382	0.8611_4^{20}	1.4958^{20}	13	138	27	v s eth; s alc; 0.02 aq
x7	Xylitol	$HOCH_2(CHOH)_3CH_2OH$	152.15	1, 531	1.52		95–97			64 aq; 1.2 EtOH; 6.0 MeOH
x8	D-(+)-Xylose		150.13	31, 47	1.535^0		156–158			117 aq; s hot alc, pyr
x9	*m*-Xylylenediamine	$C_6H_4(CH_2NH_2)_2$	136.20	13, 186	1.032	1.5709^{20}	>110			

Valeraldehyde, p28
Valeric acid, p38
Valeronitrile, p35
Valeryl chloride, p45
Vanillic acid, h143
Vanillin, h142
Vanillyl alcohol, h145
Veratraldehyde, d492
Veratric acid, d496
Veratrole, d493
Veronal, d330

Vinylacetic acid, b485
Vinylbenzene, s11
Vinyl bromide, b336
Vinyl butyl ether, b609
Vinyl chloride, c129
Vinyl cyanide, a63
Vinylethylene, b449
Vinylidene chloride, d227
Vinyltrimethylsilane, t401
Vinyltris(2-methoxyethoxy)silane, t444

Vitamin B_1, t135
Vitamin B_2, r8
Vitamin C, a302
Xanthone, x3
Xylene-α,α'-diol, b18
Xylenols, d659 thru d664
Xylidenes, d554 thru d559
o-Xylyl bromide, b443
Xylyl chlorides, c271 thru c273
p-Xylylene glycol, b19



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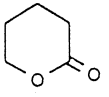

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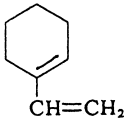

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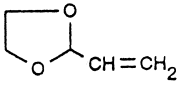

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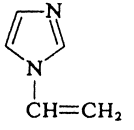

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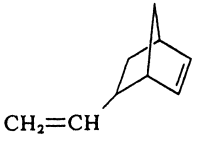

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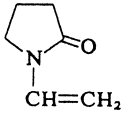

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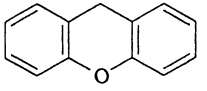
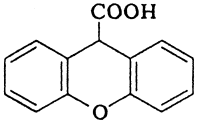
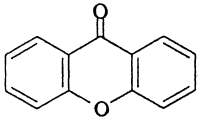


x1



x2



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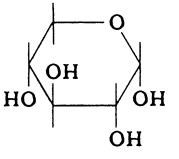

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