PHYSICAL DATA OF COMPOUNDS USED IN ORGANIC CHEMISTRY LABS

You are required to have the applicable physical data (molecular formula, molecular weight, density, melting point, boiling point, solubility properties, and hazards) for the reagents used in each experiment in this course. This data is available either in this *Handbook*, on the Internet, or in reference books.

This *Handbook* is likely to be your first choice for physical data while taking this course. The data for all the acids, bases, salts, and organic compounds used in 3321/3341 courses are given on the following pages in this Appendix.

The **Internet** currently provides a wealth of information on chemicals. For compounds not listed in this Appendix, and for more extensive information on physical and hazard information, start at the ChemInfo page on the organic chemistry website: http://orgchem.colorado.edu/cheminfo/cheminfo.html

Reference books are available at the information desk in the Science Library (in Norlin) and in the Organic Chemistry Stockroom. Three of the most useful are:

- *CRC Handbook of Chemistry and Physics* (especially Section C: "Physical Constants of Organic Compounds")
- *The Merck Index*
- *Aldrich Catalog Handbook of Fine Chemicals*

IV.1 Concentrated Acids and Bases

The physical data for the acids and bases used in organic chem lab are listed for your convenience in Table IV.1. This information was obtained in *The Chemist's Companion*, Gordon and Ford, 1972. The data is given for the most concentrated version of acid or base available, or "conc."

HAZARDS

All the concentrated acids and bases used in organic chemistry lab are corrosive enough to cause serious acid burns on the skin. The vapors can irritate the eyes and nasal passages. Handle these reagents in the main hood of the lab as much as possible. When diluted with increasing amounts of water, these reagents become less corrosive, but skin irritation will still occur upon contact.

As acids and bases are diluted, so does the IMIG/NFPA hazard rating. As a rule of thumb, for a dilution of 1:10, the hazard rating drops one value.

Table IV.1. Physical data of common acids and bases used in organic chemistry.

	Formula	**MW**	**Normality of Conc. Reag.**	**% by Weight**	**Sp. Gr.***	**Amount (mL) to Make 1 Liter of 1 N soln.**
acetic acid	CH_3CO_2H	60.05	17.4	99.8	1.05	57
hydrochloric acid	HCl	36.46	12.0	37	1.19	83
nitric acid	HNO_3	63.01	15.9	70	1.42	63
sulfuric acid	H_2SO_4	98.07	36	96	1.84	56

sodium hydroxide	NaOH	40.00	19.1	50	1.53	52
ammonia†	NH_3	17.03	14.8	29	0.90	65
phosphoric acid	H_3PO_4	97.99	14.7	85	1.70	69

* Specific gravity is the ratio of the mass of a body to the mass of an equal volume of water at 4°C. The dimensions are unity. For the purposes of the organic chemistry labs, you can estimate that specific gravity is the same as density and use the units "g/mL."

† Ammonium hydroxide.

IV.2 Salts

Useful physical data for salt solutions are listed in Table IV.2. Unless otherwise stated, the density of these solutions is about 1.0.

Table IV.2. Some properties of salts/salt solutions used in organic chemistry.

Name	Formula	MW	Solubility	Miscellaneous
copper(II) sulfate, or cupric sulfate	$CuSO_4$	159.61	60 g in 200 mL water	used to remove amines from reactions
sodium bicarbonate	$NaHCO_3$	84.00	1 part in 10 parts water at 25˚	pH of 0.1 M aq. solution = 8.3
sodium carbonate	Na_2CO_3	106.00	1 part in 3.5 parts water at 25˚	
sodium chloride	NaCl	58.45	1 gram dissolves in 2.8 mL of water at 25˚	Density of saturated solution = 1.202

The molecular weight, melting and boiling points, and density of solid inorganic drying agents (which are salts) are rarely of importance to the student of organic chemistry. In summary, these are:

- calcium chloride ($CaCl_2$)
- magnesium sulfate ($MgSO_4$)
- potassium carbonate (K_2CO_3)
- calcium sulfate ($CaSO_4$)
- sodium sulfate (Na_2SO_4)

IV.3 Organic Compounds

The physical constants contained in Table IV.4 (p. 279) were taken from the *CRC Handbook of Chemistry and Physics*, 70th Ed., 1989–1990. The hazards and toxicity data were taken from the Aldrich Catalogue (1992–1993), the *Merck Index* (10th ed.), or from the MSDS. Compounds are listed in alphabetical order according to the conventions of the CRC.

CRC CONVENTIONS

Boiling point superscripts

Boiling points with superscripts indicate the b.p. at a pressure other than atmospheric (760 mm). For example, a b.p. listed

as "245°, 128–30[10]" means that the b.p. is 245° at a pressure of 760 mm, and 128–130° at a pressure of 10 mm.

Density superscripts
"$1.011^{20/4}$" means the density of a compound taken at 20˚C relative to water at 4˚C.

Table IV.3. Abbreviations used in Table IV.4 and in the *CRC Handbook of Chemistry and Physics.*

aa	acetic acid	or	orange
ac	acid	liq	liquid
ace	acetone	mcl	monoclinic
al	alcohol	MeOH	methanol
anh	anhydrous	met	metallic
bipym	bipyramidal	monocle	monoclinic
bz	benzene	nd	needles
chl	chloroform	peth	petroleum ether
col	colorless	pl	plates
cr	crystalline	powd	powder
cub	cubic	pr	prisms
d or dec	decomposes	Py	pyrimidine
dk	dark	rh	rhombic
eth	ether	silv	silver
gr	green	tcl	triclinic
hex	hexagonal	trg	trigonal
hyg	hygroscopic	w	water
lf	leaf	wh	white
lig	ligroin	ye	yellow

SPECIAL NOTE: HYDROCARBON SOLVENTS

Hydrocarbon solvents include: petroleum ether, ligroin, Skellysolves, and hexanes. These solvents are different boiling point fractions isolated from petroleum. The longer the average hydrocarbon chain length in the mixture, the higher the boiling point. Petroleum ether is therefore not an ether at all, but a mixture of hydrocarbons with different boiling point ranges. Petroleum ethers are classified as "low-boiling range" (b.p. 30–60˚C, predominantly C_5H_{12} and C_6H_{14}) and "high-boiling range" (b.p. 60–90˚C, predominantly C_6H_{14} and C_7H_{16}). High-boiling range petroleum ether is also known as **ligroin**. The exact boiling range of ligroin depends on the supplier. Hexanes are hydrocarbons with isomers of C_6H_{14} only. Skellysolves are mixtures of saturated hydrocarbons and are classified as follows:

A: mostly *n*-pentane, b.p. range 28–38˚C.

B: mostly *n*-hexane, b.p. range 60–71˚C.

C: mostly *n*-heptane, b.p. range 88–100˚C.

D: mixed heptanes, b.p. range 80–119˚C.

In the organic chemistry teaching labs, we generally use hexanes (data in the Physical Constants Table) because, currently, they are the least expensive of the hydrocarbon solvents. Hexanes can be used interchangeably with ligroin in most experiments.

The most serious hazard associated with all the hydrocarbon solvents is their flammability, so never use them near an open flame. Breathing large volumes of their vapors can cause irritation of the respiratory tract, intoxication, and depression of the central nervous system. Too much skin contact can cause irritation.

Table IV.4. Physical constants and hazards of some organic and inorganic compounds.

	Mol. Wt.	Color, Cryst. form	b.p. ˚C	m.p. ˚C	Density	Solubility	Hazards	Toxicity
Acetanilide or N-phenylacetamide, $CH_3CONHC_6H_5$	135.17	rh or pl (w)	304	114.3	1.2190^{15}	al, eth, ace, bz	toxic, irritant	LD_{50} (rats, oral): 1930 mg/kg; general narcotic action in humans, large doses may cause death by respiratory paralysis.
Acetanilide, p-hydroxy or p-acetamidophenol, 4-$HOC_6H_4NHCOCH_3$	151.17	nd (bz-peth)	.....	169–172	.....	al, eth, bz	toxic, irritant	LD_{50} (mice, oral): 338 mg/kg
Acetic acid (see p. 276)								
Acetic acid, 3-methyl butyl ester or iso-pentyl acetate or iso-amyl acetate, $CH_3CO_2CH_2CH_2CH(CH_3)_2$	130.19	.....	142	–78.5	$0.8670^{20/4}$	al, eth, ace	flammable liquid, irritant	LD_{50} (rats, oral): 16600 mg/kg
Acetic acid, anhydride, or acetic anhydride, $(CH_3CO)_2O$	102.09	.....	139.55, 44^{15}	–73.1	$1.0820^{20/4}$	al, eth, bz, w	corrosive, lachrymator	LD_{50} (rats, oral): 1.78 g/kg. Produces irritation and necrosis of tissues.
Acetic acid, butyl ester or butyl acetate, $CH_3CO_2C_4H_9$	116.16	.....	126.5	–77.9	$0.8825^{20/4}$	al, eth, bz	flammable liquid, irritant	LD_{50} (rats, oral): 14.13 g/kg; narcotic to humans in high concentrations
Acetic acid, ethyl ester or ethyl acetate, $CH_3CO_2C_2H_5$	88.11	.....	77.06	–83.6	$0.9003^{20/4}$	w, al, eth, ace, bz	flammable, irritant	LD_{50} (rats, oral): 11.3 mL/kg
Acetic acid, octyl ester or octyl acetate, $CH_3CO_2C_8H_{17}$	172.27	.....	210, $112–3^{30}$	–38.5	$0.8705^{20/4}$	al, eth		LD_{50} (rats, oral): 3.0 g/kg
Acetonaphthone, 2', $C_{10}H_7COCH_3$	170.21	white	300–1	53–5			irritant	LD_{50} (oral, mus): 599 mg/kg
Acetone or 2-Propanone, CH_3COCH_3	58.08	.....	56.2	–95.35	$0.7899^{20/4}$	w, al, eth, bz, chl	flammable, irritant	inhalation TLC_{LO}, 500 ppm
acetonitrile, CH_3CN	41.05	.....	81.6	–45.7	0.7857^{20}	w, al, eth, ace, bz	highly flammable, harmful, irritant, possible carcinogen	LD_{50} (rats, oral) 2460 mg/kg; LC_{50} (rats, inhalation) 7,551 ppm
Acetophenone or methyl phenyl ketone, $C_6H_5COCH_3$	120.15	mcl pr or pl	202.6, 79^{10}	20.5	$1.0281^{20/4}$	al, eth, ace, bz, chl	harmful, irritant	LD_{50} (rats, oral): 815 mg/kg
Acetophenone, 4-bromo or 4-bromo phenyl methyl ketone, 4-$BrC_6H_4COCH_3$	199.05	lf (al)	255.5^{736}, 130^{11}	50–1	1.647	al, eth, bz, aa	harmful, irritant	

	Mol. Wt.	Color, Cryst. form	b.p. ˚C	m.p. ˚C	Density	Solubility	Hazards	Toxicity
Acetophenone, 4-methoxy, 4-$CH_3OC_6H_4COCH_3$	150.18	.....	258, 138–9[15]	38–9	1.0818[41/4]	al, eth, ace	harmful, irritant	LD_{50} (rats, oral): 1720 mg/kg
Acetophenone, 4-methyl or 4-acetyl toluene, 4-$CH_3C_6H_4COCH_3$	134.18	nd	226, 113[11]	28	1.0051[20/4]	al, eth, bz	harmful	LD_{50} (rats, oral): 1400 mg/kg
Acetylferrocene, $C_{12}H_{12}OFe$	228.07	.....	.....	81–83	.....	.....	highly toxic	
Aluminum chloride, $AlCl_3$	133.34	wh to col, hex	d 262, 182.7[752], subl.177.8	190[2.5]	.....	w, al, CCl_4, eth	corrosive, moisture sensitive	LD_{50} (rats, oral): 3730 mg/kg; anhydrous form is a strong irritant
Ammonium cerium (IV) nitrate, (ceric ammonium nitrate), $(NH_4)_2Ce(NO_3)_6$	548.23	or, monocle	.....	.....	.....	w, ace, al	oxidizer, irritant	
Ammonium formate, HCO_2NH_4	63.06	wh, monocl, deliq	180 d	116	1.280	w, al, eth, NH_3	irritant, hygroscopic	.....
Ammonium hydroxide (see p. 276)								
Aniline or phenylamine, $C_6H_5NH_2$	93.13	.....	184, 68.3[10]	–6.3	1.02173[20/4]	al, eth, ace, bz, lig	highly toxic, irritant	Intoxication may occur from inhalation, ingestion, or cutaneous absorption.
Aniline, 4-bromo, 4-Br-$C_6H_4NH_2$	172.02	rh bip yrm nd (60% al)	d	66.4	1.4970[100/4]	al, eth	toxic, irritant	
Aniline, 2-nitro, 2-$(NO_2)C_6H_4NH_2$	138.13	gold-ye pl or nd	284, 165–6[28]	71.5	1.442[15]	al, eth, ace, bz	highly toxic, irritant	
Aniline, 4-nitro, 4-$(NO_2)C_6H_4NH_2$	138.13	pa ye mcl nd (w)	331.7, 106[0.03]	148–9	1.424[20/4]	al, eth, ace, chl	highly toxic, irritant	
Anisic acid, p-, or 4-methoxybenzoic acid, 4-$(CH_3O)C_6H_4CO_2H$	152.15	nd (w)	170–2[10]	184	.....	al, eth, bz	.....	
Anthracene, 9-hydroxymethyl, or 9-anthracenemethanol, $C_{15}H_{12}O$	208.26	ye, ye/or		162–4	.....		possible irritant	
Benzaldehyde, C_6H_5CHO	106.12	.....	178, 62[10]	–26(fr–56)	1.0415[10/4]	al, eth, ace, bz, lig	harmful	LD_{50} (rats, oral): 1300 mg/kg Remarks: Behavioral: Somnolence (general depressed activity). Behavioral: Coma.

	Mol. Wt.	Color, Cryst. form	b.p. ˚C	m.p. ˚C	Density	Solubility	Hazards	Toxicity
Benzaldehyde, 2-chloro, 2-ClC_6H_4CHO	140.57	nd	211.9, 84.3[10]	12.4	1.2483[20/4]	al, eth, ace, bz	corrosive	LD_{50} (rats, oral): 2160 mg/kg Somnolence. Hypermotility, diarrhea. Tremor.
Benzaldehyde, 3-chloro, 3-ClC_6H_4CHO	140.57	pr	213–4, 55[1]	17–8	1.2410[20/4]	al, eth, ace, bz	irritant	
Benzaldehyde, 4-chloro, 4-ClC_6H_4CHO	140.57	pl	213–4, 72–5[3]	47.5	1.196[61/4]	w, al, eth, ace, bz	harmful, irritant	LD_{50} (rats, oral): 1575 mg/kg Behavioral:Altered sleep time. Somnolence. Excitement.
Benzaldehyde, 3,4-dimethoxy, 3,4-$(CH_3O)_2C_6H_3CHO$	166.18	nd (eth, lig, to)	258, 172–5[18]	44 (58)	.....	al, eth	irritant	LD_{50} (rats, oral): 1300 mg/kg
Benzaldehyde, 2-methoxy or o-Anisaldehyde, 2-$CH_3OC_6H_4CHO$	136.15	pr	243–4, 124–5[18]	37–8	1.1326[20/4]	al, eth, ace, bz, chl	irritant	LD_{50} (rats, oral): 2500 mg/kg
Benzaldehyde, 4-methoxy or p-Anisaldehyde, 4-$CH_3OC_6H_4CHO$	136.15	.....	249.5, 83[2]	0	1.1191[15/4]	al, eth, ace, bz	harmful, irritant	LD_{50} (rats, oral): 3210 mg/kg
Benzaldehyde, 4-methyl or p-Tolualdehyde, 4-$CH_3C_6H_4CHO$	120.15	.....	204–5, 106[10]	.....	1.0194[17/4]	al, eth, ace, chl	harmful, irritant	LD_{50} (rats, oral): 1600 mg/kg Behavioral: Somnolence.
Benzaldehyde, 2-nitro, 2-$NO_2C_6H_4CHO$	151.12	ye nd (w)	153[23]	43.5–44	1.2844[20/4]	al, eth, ace, bz	irritant	
Benzaldehyde, 3-nitro, 3-$NO_2C_6H_4CHO$	151.12	lt ye nd (w)	164[23]	58	1.2792[20/4]	al, eth, ace, bz	irritant	
Benzene, 1,4-di-tert-butyl or p-di-tert-butyl benzene, 1,4-$[(CH_3)_3C]_2C_6H_4$	190.33	nd (MeOH)	237[743], 109[15]	80–1	.....	al, eth	flammable liquid	
Benzene, bromo or phenylbromide, C_6H_5Br	157.01	.....	156, 43[18]	–30.8	1.4950[20/4]	al, eth, bz	irritant	
Benzene, ethyl or Ethylbenzene, $C_6H_5C_2H_5$	106.17	.....	136.2, 25.8[10]	–95	0.8670[20/4]	al, eth	flammable, irritant	LD_{50}(rats, oral): 5.46 g/kg
Benzene, nitro, $C_6H_5NO_2$	123.11	.....	210.8	5.7	1.2037[20/4]	al, eth, ace, bz	highly toxic, irritant	Rapidly absorbed through skin, vapor hazardous. May cause headaches, drowsiness, nausea, vomiting, methemoglobinemia with cyanosis.

	Mol. Wt.	Color, Cryst. form	b.p. ˚C	m.p. ˚C	Density	Solubility	Hazards	Toxicity
Benzene, tert-butyl, $C_6H_5C(CH_3)_3$	134.22	.....	169, 50.7[10]	–57.8	$0.8665^{20/4}$	al, eth, ace, bz	flammable	
Benzenesulfonamide, 4-acetamido, 4-(CH_3CONH)-$C_6H_4SO_2NH_2$	214.24	nd (aa)	.....	219–20	.....	w, al, ace	irritant	
Benzenesulfonyl chloride, 4-acetamido, 4-$(CH_3CONH)C_6H_4SO_2Cl$	233.67	nd (bz), pr (bz-chl)	.....	149	.....	al, eth	corrosive, moisture-sensitive	
Benzhydrol or diphenylmethanol, $(C_6H_5)_2CHOH$	184.24	nd (lig)	297–8[748], 180[20]	69	.....	al, eth	irritant	
Benzil or diphenyl-glyoxal, $C_6H_5COCOC_6H_5$	210.23	ye pr (al)	346–8d, 188[12]	95–6	$1.084^{102/4}$	al, eth, ace, bz	irritant	LD_{50} (oral, mus): >3 gm/kg
Benzoic acid, 3-chloro, 3-$ClC_6H_4CO_2H$	156.57	pr (w)	sub	158	$1.496^{25/4}$	al, eth	irritant	
Benzoic acid, $C_6H_5CO_2H$	122.12	mcl lf or nd	249, 133[10]	122.13	$1.2659^{15/4}$	al, eth, ace, bz, chl	irritant	
Benzoic acid, methyl ester or methyl benzoate, $C_6H_5CO_2CH_3$	136.15	.....	199.6, 96–8[24]	–12.3	$1.0888^{20/4}$	al, eth, MeOH	irritant	LD_{50} (rats, oral): 3.43 g/kg
Benzophenone or diphenyl ketone, $C_6H_5COC_6H_5$	182.22	rh pr (al, eth)	305.9	48.1	1.146^{20}	al, eth, ace, bz	irritant	
Benzoquinone, 1,4-, or p-quinone, $C_6H_4(=O)_2$	108.10	ye mcl pr (w)	sub	113–5	1.318^{20}	al, eth	highly toxic, flammable, irritant	LD_{50} (rats, oral):130 mg/kg
Benzyl chloride or □-chlorotoluene, $C_6H_5CH_2Cl$	126.59	.....	179.3, 6611	–39	$1.1002^{20/20}$	al, eth, chl	highly toxic, cancer suspect agent	irritant; very large doses causes CNS depression
Biphenyl or phenylbenzene, C_6H_5-C_6H_5	154.21	lf (dil al)	255.9, 145[22]	71	$0.8660^{20/4}$	al, eth, bz	irritant	LD_{50} (rats, oral): 3280 mg/kg; CNS depression, paralysis, convulsions observed in exptl animals
Biphenyldimethanol, 2,2'-, $-(C_6H_4CH_2OH)_2$	214.26	wh		110–1			possible irritant	
Biphenylmethanol, 4-, $C_6H_5C_6H_4CH_2OH$	184.24	wh		99–101			possible irritant	
Bromine, Br_2	159.8	dk red liq	58.78	–7.2	3.119	al, eth, chl	highly toxic, oxidizer	

	Mol. Wt.	Color, Cryst. form	b.p. ˚C	m.p. ˚C	Density	Solubility	Hazards	Toxicity
1,3, Butadiene,1,4-diphenyl (trans, trans), $C_6H_5CH=CH–CH=CHC_6H_5$	206.29	lf (al or aa)	350^{720}	152.5	.....	al, eth, bz, chl, peth	irritant	
Butanol, 1- or n-butyl alcohol, $CH_3CH_2CH_2CH_2OH$	74.12	.....	117.2	–89.5	$0.8098^{20/4}$	w, al, eth, ace, bz	flammable liquid	LD_{50} (rats, oral): 4.36 g/kg; may cause irritation of mucous membranes, contact dermatitis, headache, dizziness, drowsiness.
Butanol, 1-, 3-methyl or iso-amyl alcohol, $(CH_3)_2CHCH_2CH_2OH$	88.15	.....	128.5^{750}	–117.2	$0.8092^{20/4}$	al, eth, ace	irritant	LD_{50} (rats, oral): 7.07 mL/kg
2-Butanone, 3-hydroxy-3-methyl, $(CH_3)_2COHCOCH_3$	102.13	.....	140–1	.....	0.971	.....		
Butyl alcohol, tert- or 2-Methyl-2-propanol, $(CH_3)_3COH$	74.12	.....	82.3, 20^{31}	25.5	$0.7887^{20/4}$	w, al, eth	flammable, irritant	LD_{50}(rats, oral): 3.5 g/kg
Butyl chloride, tert- or 2-Chloro-2-methyl propane, $(CH_3)_3CCl$	92.57	.....	51–52	–25.4	$0.8420^{20/4}$	al, eth, bz, chl	flammable	
3-Butyn-2-ol, 2-methyl, $(CH_3)_2COHC{\equiv}CH$	84.12	.....	104, 56^{97}	+3	$0.8618^{20/4}$	w, al	flammable liquid, toxic	LD_{50} (mice, i.p.): 3.6 g/kg
Butyryl chloride, 3-methyl, or isovaleryl chloride, $(CH_3)_2CHCH_2COCl$	120.58	.....	110–3	.....	0.982	eth	flammable, corrosive, irritant, lachrymator, reacts violently with water	
Caffeine or 1,3,7-Trimethylxanthine, $C_8H_{10}N_4O_2$	194.19	wh nd (w+l), hex pr (sub)	sub 178, sub 89^{15}	238 (anh)	1.23^{19}	py, chl	toxic	LD_{50} (mice, hamsters, rats, rabbits, oral, mg/kg): 127, 230, 355, 246 (males); 137, 249, 247, 224 (females)
Carotene, □-, $C_{40}H_{56}$	536.88	red br hex pr (bz-MeOH)	.....	184	$1.00^{20/20}$	eth, ace, bz, peth	.....	
Chlorophyll a, $C_{55}H_{72}MgN_4O_5$	893.51	bl bk hex pl	.....	150–3	.....	al, eth, lig	.....	
Chlorophyll b, $C_{55}H_{70}MgN_4O_5$	907.49	bl bk gr pw	.....	120–30	.....	al, eth, lig		

	Mol. Wt.	Color, Cryst. form	b.p. ˚C	m.p. ˚C	Density	Solubility	Hazards	Toxicity
Chlorosulfonic acid, $ClSO_3H$	116.52	.....	158	–80	1.766^{18}	d to $H_2SO_4^+$ in water	highly toxic, oxidizer	extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin
Cholesterol, $C_{27}H_{45}OH$	386.66	rh or tcl lf (al+1w), nd(eth)	360d, $233^{0.5}$	148.5 (anh)	$1.067^{20/4}$	eth, bz, peth		
Cinnamaldehyde, trans, $C_6H_5CH{=}CHCHO$	132.16	yesh	253d, 127^{16}	–7.5	$1.0497^{20/4}$	al, eth, chl	irritant	
Cinnamic acid, trans-, $C_6H_5CH{=}CHCO_2H$	148.16	mcl pr (dil al)	300 (cor)	135–6	$1.2475^{4/4}$	al, eth, ace, bz, chl	irritant	
Cumene or iso-Propylbenzene, $(CH_3)_2CHC_6H_5$	120.19	.....	152.4, 38.2^{10}	–96	$0.8618^{20/4}$	al, eth, ace, bz	irritant	LD_{50}(rats, oral): 1.4 g/kg
Cyclohexane, C_6H_{12}	84.16	.....	80.7	6.5	$0.7785^{20/4}$	al, eth, ace, bz, lig	flammable, irritant	LD_{50} (rat, oral): 12.7 g/kg
Cyclohexane, methyl or Hexahydrotoluene, $CH_3C_6H_{11}$	98.19	.....	100.9, 16.3^{10}	–126.6	$0.7694^{20/4}$	al, eth, ace, bz	flammable, irritant	
Cyclohexanol, $C_6H_{11}OH$	100.16	hyg nd	161.1	25.1	$0.9624^{20/4}$	w, al, ace, eth, bz	irritant, hygroscopic	LD_{50} (rats, oral): 2.06 g/kg
Cyclohexanol, 2-methyl, 2-$CH_3C_6H_{10}OH$	114.19	.....	166, 78^{20}	.....	0.9454^{20}	al, eth	irritant	TLV (human): 50 ppm
Cyclohexanone, $C_6H_{10}O$	98.14	.....	155.6, 47^{15}	–26.4	$0.9478^{20/4}$	al, eth, ace, bz, chl	corrosive, toxic	LD_{50} (rats, oral): 1.62 mL/kg
Cyclohexene, C_6H_{10}	82.15	.....	83	–103.5	$0.8102^{20/4}$	al, eth, ace, bz	flammable, irritant	LD_{50} (rats, oral): 2400 UL/kg
Cyclohexene, 1-methyl, 1-$CH_3C_6H_9$	96.17	.....	110, 24.6^{30}	–121	$0.8102^{20/4}$	eth, bz	flammable, irritant	
Cyclohexene, 3-methyl, 3-$CH_3C_6H_9$	96.17	.....	104	–115.5	$0.7990^{20/4}$	eth, bz, peth, chl		
Cyclopentadiene, C_5H_6	66.10	.....	40.0	–97.2	$0.8021^{20/4}$	al, eth, ace, bz	.....	LD_{50} (rats, oral): .82 g/kg
Diacetylferrocene, $C_{14}H_{14}O_2Fe$	270.11	.....	.....	125–7	.....	.....	.....	
Dicyclopentadiene, $C_{10}H_{12}$	132.21	.....	170	–1	0.986	al, eth, aa	flammable liquid, toxic	
Dimethoxybenzyl alcohol, 2,5-, $(CH_3O)_2C_6H_3CH_2OH$	168.19	.....	99–$101^{0.2}$	.....	1.168	irritant		

	Mol. Wt.	Color, Cryst. form	b.p. ˚C	m.p. ˚C	Density	Solubility	Hazards	Toxicity
Dimethoxybenzyl-3-methylbutanoate, 2,5-, $C_{14}H_{20}O_4$	252.31		$131.5^{0.5}$	.....	not yet determined		unknown	unknown
Epoxycholestan-3□-ol, 5□, 6□-, $C_{27}H_{44}O_2$	402.66	.....	.....	139–41	.....	.....	.....	
Ethanol or ethyl alcohol, CH_3CH_2OH	46.07	.....	78.5	–117.3	$0.7893^{20/4}$	w, eth, ace, bz	highly toxic, flammable	LD_{50} (oral, rat): 13.0 mL/kg LD_{Lo} (human, oral): 1.4 g/kg
Ethyl ether or diethyl ether, $C_2H_5OC_2H_5$	74.12	.....	34.5	–116.2	$0.7138^{20/4}$	al, ace, bz, chl	flammable, irritant	LD_{50} (rats, oral): 2.2 g/kg
Ferrocene, $C_{10}H_{10}Fe$	186.04	.....	249	172.5	.....	.....		
Fluorene or 2,3-Benzindene, $C_{13}H_{10}$	166.22	lf (al)	293–5	116–7	$1.203^{0/4}$	eth, ace, bz	.....	
Fluorenemethanol, 9-, $C_{14}H_{12}O$	196.25	off-white to ye		105–7			possible irritant	
Fluorenone, 9-, $C_{13}H_8O$	180.21	ye rh bipym (al, bz-peth)	342	82–5	$1.1300^{99/4}$	al, eth, ace, bz	possible irritant	LD_{50} (ipr, mus): >2 gm/kg
Formamide, N,N-dimethyl, $HCON(CH_3)_2$	73.09	.....	149–56, 39.9^{10}	–60.5	$0.9487^{20/4}$	w, al, eth, ace, bz, chl	cancer suspect agent, irritant	vapor harmful; irritating to skin, eyes, and mucous membranes
Fumaric acid, dimethyl ester or Dimethyl fumarate, $CH_3O_2CCH{=}CHCO_2\text{-}CH_3$	144.13	.....	193	103–4	$1.37^{20/4}$	ace, chl	irritant	LD_{50} (oral, rat): 2.24 g/kg
Gentisyl quinone isovalerate, or blattellaquinone, $C_{12}H_{14}O_4$	222.24	golden brn (eth/pet eth)		56.5˚	.....		harmful	unknown
Heptaldehyde, $CH_3(CH_2)_5CHO$	114.19	.....	152.8, 59.6^{10}	–43.3	$0.8495^{20/4}$	al, eth	irritant	LD_{50} (rats, oral): 3200 mg/kg Remarks: Behavioral: Muscle weakness.
Heptanone, 4- or depropyl ketone, $(C_3H_7)_2CO$	114.19	.....	144	–33	$0.8174^{20/4}$	al, eth	flammable, harmful	LD_{50} (rats, oral): 3730 mg/kg
Hexane-1,6-diamino or hexamethylene diamine, $H_2N(CH_2)_6NH_2$	116.21	rh bipym pl	204–5, 100^{20}	41–2	.....	w, al, bz	corrosive, hygroscopic	
Hexanes, C_6H_{14}	86.18	.....	69	–95	0.655	al, eth, chl	flammable, irritant	

	Mol. Wt.	Color, Cryst. form	b.p. ˚C	m.p. ˚C	Density	Solubility	Hazards	Toxicity
Hydrazine, 2,4-dinitrophenyl, $[2,4\text{-}(O_2N)_2C_6H_3]NHNH_2$	198.14	blsh-red (al)	.....	194, (198d)	.....	.....	flammable solid, irritant	
Ibuprofen, $(CH3)_2CHCH_2C_6H_4\text{-}CH\text{-}(CH_3)CO_2H$	206.27	.....	.....	75–77	.....	al, eth, ace	toxic	LD_{50} (mice, oral): 1255 mg/kg
Indanol, 2-, $C_9H_{10}O$	134.18	tan		68–71			possible irritant	
Indanone, 1-, C_9H_8O	132.16	ta, nd, off-white	241–2[739], 129[12]	40–42	1.1028[40/40]	al, eth, ace, chl, lig	possible irritant	
Indigo, $C_{16}H_{10}N_2O_2$	262.27	.....	.....	390–2d	1.35	.....	irritant	
Limonene (d) or 4-isopropenyl-1-methyl cyclohexene, $C_{10}H_{16}$	136.24	$[\sigma]^{20/D}$ +125.6 (undil)	178, 61[12]	–74.3	0.8411[20/4]	al, eth	harmful, irritant	LD_{50} (oral, rat): 4400 mg/kg Remarks: Behavioral: Change in motor activity (specific assay). Lungs, Thorax, or Respiration: Respiratory depression.
Magnesium, Mg	24.3050	silv wh met, hex	1107	648.8	1.745	.....		Particles embedded in skin can produce gaseous blebs. Inhalation of dust is irritating.
Maleic acid, dimethyl ester or Dimethyl maleate, $CH_3O_2CCH{=}CHCO_2CH_3$	144.13	.....	202, 102[17]	–19	1.1606[20/4]	eth	toxic, irritant	LD_{50} (oral, rat): 1.41 g/kg
Maleic anhydride, $C_4H_2O_3$	98.06	nd (chl eth)	197–9, 82[14]	60	1.314[60]	eth, ace, chl	corrosive, toxic	Powerful irritant; avoid contact with skin, eyes, clothing. Avoid inhalation.
Mercury (II) oxide or mercuric oxide, HgO	216.59	yel or red, rhomb	.....	d 500	1.1[4]	acid	highly toxic, irritant	poison
Methane, dichloro or Methylene chloride, CH_2Cl_2	84.93	.....	40	–95.1	1.3266[20/4]	al, eth	toxic, irritant	LD_{50} (rats, oral): 1.6 mL/kg; Narcotic to humans in high concentration; TC_{Lo} (humans): 500 ppm
Methane, diphenyl, $(C_6H_5)_2CH_2$	168.24	pr nd	264.3, 125.5[10]	25.3	1.0060[20/4]	al, eth, chl	.....	.....
Methane, tetrachloro or Carbon tetrachloride, CCl_4	153.82	.....	76.5	–23	1.5940[20/4]	al, eth, ace, bz, chl	cancer suspect agent, toxic	inhalation TC_{LO}, 20 ppm
Methane, trichloro or Chloroform, $CHCl_3$	119.38	.....	61.7	–63.5	1.4832[20/4]	al, eth, ace, bz, lig	highly toxic, cancer suspect	inhalation TC_{LO}, 10 ppm

	Mol. Wt.	Color, Cryst. form	b.p. ˚C	m.p. ˚C	Density	Solubility	Hazards	Toxicity
Methanol or Methyl alcohol, CH_3OH	32.04	.....	65, 15[73]	–93.9	$0.7914^{20/4}$	w, al, eth, ace, bz, chl	flammable, poisonous	inhalation TC_{Lo}, 300 ppm (humans)
Naphthalene, $C_{10}H_8$	128.17	mcl pl (al)	218, 87.5[10]	80.5	$0.9625^{100/4}$, 1.0253^{20}	al, eth, ace, bz	flammable, toxic	poisonous to humans in large doses
Naphthalenemethanol, 1-, $C_{10}H_7CH_2OH$	158.20	nd (w, al) cr (bz-liq), off-white	301[715], 163[12]	61–3	$1.1039^{20/4}$	al, eth		LD_{50} (skin, rats): >5 g/kg
Naphthoquinone, 1,4-, $C_{10}H_6O_2$	158.16	bt ye nd (al peth) ye (sub)	sub	123	.....	al, eth, bz, aa	highly toxic, irritant	LD_{50} (rats, oral): 190 mg/kg
Nitric acid (see p. 87)								
Nitrobenzoic acid, 3-, methyl ester, $3\text{-}NO_2C_6H_4CO_2CH_3$	181.15	nd	.....	78	.....	.....	may cause irritation	
Norbornene-, cis-5-, endo-2,3-dicarboxylic anhydride	164.16	.....	.....	165–7	.....	.....	flammable, moisture sensitive	
Octanol, 1- or octyl alcohol, $CH_3(CH_2)_6CH_2OH$	130.23	.....	194.4, 98[19]	–16.7	$0.8270^{20/4}$	al, eth	irritant	LD_{50} (oral, mus): 1.79 g/kg
Octanone, 2- or methyl hexyl ketone, $C_6H_{13}COCH_3$	128.21	.....	173, 59–60[11]	–16	$0.8202^{20/4}$	al, eth	harmful	LD_{50} (rats, oral): 3089 mg/kg
Palladium on activated carbon, Pd-C (10% Pd)							flammable solid	
Pentane, $CH_3(CH_2)_3CH_3$	72.15	.....	36.1	–130	$0.6262^{20/4}$	al, eth, ace, bz, chl	flammable, irritant	LD_{Lo} (mice, inhalation): 128,200 ppm
2-Pentanone, 4-methyl or methyl isobutyl ketone, $(CH_3)_2CHCH_2COCH_3$	100.16	.....	116.8, 35–40[16]	–84.7	0.7978^{20}	al, eth, ace, bz, chl	flammable, harmful	LD_{50} (rats, oral): 2080 mg/kg
Peroxybenzoic acid, 3-chloro, $3\text{-}ClC_6H_4COOOH$	172.57	.....	.....	92–4 dec	.....	.....	oxidizer, irritant	
Phenanthrene, $C_{14}H_{10}$	178.23	mcl pl (al), lf (sub)	340, 210–15[12]	101	0.9800^{4}	al, eth, ace, bz, aa	irritant	LD_{50} (rats, oral): 700 mg/kg
Phenyl acetic acid, $C_6H_5CH_2CO_2H$	136.15	lf, pl (peth)	265.5, 144–5[12]	77	$1.091^{77/4}$, 1.228^{6}	al, eth, ace	irritant	LD_{50} (rats, oral): 2250 mg/kg
Phenylcyclohexanone, 4-, $C_6H_5C_6H_9(=O)$	174.24	white		78–80			possible irritant	
3-Phenylpropanoic acid, erythro-2,3-dibromo, $C_9H_8O_2Br_2$	308.8	.....	.....	202–4	.....	.....		

	Mol. Wt.	Color, Cryst. form	b.p. ˚C	m.p. ˚C	Density	Solubility	Hazards	Toxicity
3-Phenylpropanoic acid, threo-2,3-dibromo, $C_9H_8O_2Br_2$	308.0	.....	.....	93.5–95	.....	.....		
Phosphoric acid, H_3PO_4 (see p. 280)								
Phosphorous acid, triethyl ester or triethyl phosphite, $(C_2H_5O)_3P$	166.16	.....	157.9, 49[12]	.....	$0.9629^{20/4}$	.....	irritant	
Propionic acid or propanoic acid, $CH_3CH_2CO_2H$	74.08	.....	141, 41.6[10]	–20.8	0.9930^{20}	w, al, eth	corrosive, toxic	LD_{50} (rats, oral): 4.29 g/kg
Propionic acid, butyl ester or butyl propionate, $CH_3CH_2CO_2C_4H_9$	130.19	.....	145.5	–89.5	$0.8754^{20/4}$	al, eth	irritant	LD_{50} (rats, oral): 5 g/kg
Propiophenone, or ethyl phenyl ketone, $C_6H_5COC_2H_5$	134.18	.....	217.5, 91.6[10]	18.6	1.0096^{20}	al, eth	irritant	LD_{50} (rats, oral): 4490 microL/kg
pyridine, C_5H_5N	79.10	.....	115	–42	0.978	w, al, eth, ace, bz	flammable, irritant, possible carcinogen, readily absorbed through skin	LD_{50} (rats, oral) 891 mg/kg; LD_{50} (rabbits, skin) 1,121 mg/ kg; LC_{50} (rats, inhalation) 9,015 ppm
Salicylic acid acetate or Aspirin, 2-$CH_3CO_2C_6H_4CO_2H$	180.16	nd (w), mcl ta p	135	.....	al, eth, chl	.....	.....	
Sebacoyl chloride, $ClOC(CH_2)_8COCl$	239.14	.....	220[75], 165[11]	–2.5	$1.1212^{20/4}$	.....	corrosive, lachrymator	
Sodium bicarbonate, $NaHCO_3$ (see also p. 280)	84.01	wh, monocle pr	.....	.....	2.159	w, al	.....	
Sodium bisulfite, $NaHSO_3$	104.06	wh, monocle	.....	d	1.48	w, al	corrosive	LD_{50} (rats, i.v.): 115 mg/kg; concentrated solutions are irritating to skin, mucous membranes
Sodium borohydride, $NaBH_4$	37.83	white cub	.....	400 dec	1.074	w, al	flammable solid, corrosive	
Sodium carbonate, Na_2CO_3	105.99	wh powd	d	851	2.532	w, al	irritant, hygroscopic	concentrated solns in contact with skin or eyes may cause local necrosis

	Mol. Wt.	Color, Cryst. form	b.p. ˚C	m.p. ˚C	Density	Solubility	Hazards	Toxicity
Sodium chloride (see also p. 276)	58.44	col, cub	.....	801	$2.165^{25/4}$	w, al	.....	
Sodium hydrosulfite or sodium dithionite, $Na_2S_2O_4$	174.11	col, monocle cr	.....	>300 dec	.....	w	flammable solid, moisture sensitive	
Sodium hydroxide (see p. 276)								
Sodium hypochlorite, NaOCl	74.44	found only in solution	.....	.....	.....	.....	oxidizer, corrosive	Ingestion may cause corrosion of mucous membranes; inhalation may produce bronchial irritation; skin irritant.
Sodium methoxide, $NaOCH_3$	54.02	wh powd	.....	.....	.....	w, al	flammable solid, corrosive	
Sodium thiosulfate, $Na_2S_2O_3$	158.11	col, monocle	.....	.....	1.667	w	irritant	
Stilbene, trans-, or trans-1,2-diphenylthylene, $C_6H_5CH{=}CHC_6H_5$	180.25	cr (al)	305^{720}, $166–7^{12}$	124–5	0.9707	eth, bz	.....	
Succinic acid, $HO_2CH_2CH_2CO_2H$	118.09	tcl or mcl pr	235d	188	$1.572^{25/4}$	al, eth, ace	irritant	LD_{50} (rats, oral): 2260 mg/kg
Sulfanilamide or 4-aminobenzene sulfonic acid, $4\text{-}H_2NC_6H_4SO_2NH_2$	172.20	lf (aq al)	.....	165–6	1.08	al, eth, ace	irritant	LD_{50} (dogs, oral): 2.0 g/kg
Sulfuric acid (see p. 276)								
Thymol blue or thymolsulfonephthalein, $C_{27}H_{30}O_5S$	466.59	gr-red (al, eth, aa)	.....	221-4d	.....	al, aa	.....	
Tin, Sn	118.69	gray, cub	2270	231.968	5.75	acid	.....	
Toluene or Methyl benzene, $C_6H_5CH_3$	92.14	.....	110.6, $14.5^{14.5}$	–95	$0.8669^{20/4}$	al, eth, ace, bz, lig	flammable, toxic	LD_{50} (rats, oral): 7.53 g/kg
Triethyl phosphite: see Phosphorous acid, triethyl ester								
Triphenylmethanol or tritanol, $(C_6H_5)_3COH$	260.34	pl (al), trg (bz)	380	164.2	$1.199^{0/4}$	al, eth, ace, bz, aa		