

APPENDIX

Tables of Unknowns and Derivatives

The following tables list several hundred organic compounds and provide representative examples of the six functional-group classes that are treated in Part 4, Organic Qualitative Analysis. The functional groups appear in alphabetical order in Tables 1–7. In each table, compounds are listed in order of increasing boiling points; solids appear last in each table in order of increasing melting points. Compounds are arbitrarily listed by increasing boiling points unless their melting points are above 40°C. Many pure compounds that melt just above room temperature may be in the liquid state when you encounter them due to depression of their melting points by impurities. Remember also that the melting points we list may be 2°–3°C higher or even more than the values you measure, because the listed melting points are those of the purified compounds.

When a derivative has been reported to decompose on melting, a "d" marks the melting point. When no solid derivative is listed in standard reference tables for an alcohol, aldehyde, ketone, amine, carboxylic acid, or phenol, a dash appears in the table in place of the derivative's melting point. In a few cases, two widely different melting points for a compound are listed in the literature; we include both, the second one in parentheses. The derivatives of multifunctional compounds that can form through derivatization at more than one site are shown by the notation "(mono)," "(di)," or "(tri)" after the melting point.

TABLE 1 Alcohols

Compound	bp, °C	mp, °C	3,5-Dinitrobenzoate	1-Naphthylurethane	Phenylurethane
Methanol	65		107	124	47
Ethanol	78		93	79	52
2-Propanol	83		122	106	76
2-Methyl-2-propanol	83	25	142	101	136
2-Propen-1-ol	97		49	108	70
1-Propanol	97		74	80	57
2-Butanol	99		75	97	65
2-Methyl-2-butanol	102		116	72	42
2-Methyl-1-propanol	108		86	104	86
1-Butanol	116		64	71	61
3-Pentanol	116		99	95	48
2-Pentanol	119		61	74	—
3-Methyl-3-pentanol	123		96 (62)	83	43
2-Methoxyethanol	124		—	112	—
1-Chloro-2-propanol	127		77	—	—
2-Methyl-1-butanol	129		70	82	31
3-Methyl-1-butanol	131		61	68	55
2-Chloroethanol	131		95	101	51
4-Methyl-2-pentanol	132		65	88	143
2-Ethoxyethanol	135		75	67	—
3-Hexanol	135		97 (77)	—	—
1-Pentanol	138		46	68	46
2-Hexanol	139		38	60	—
Cyclopentanol	140		115	118	132
3-Hydroxy-2-butanone	145		—	—	—
2,2,2-Trichloroethanol	151	19	142	120	87
1-Hexanol	157		58	60	42
2-Heptanol	159		49	54	—
Cyclohexanol	161	25	112	129	82
1-Amino-2-propanol	163		—	—	—
4-Hydroxy-4-methyl- 2-pentanone	166		55	—	—
2-Furylmethanol	171		80	130	45
1-Heptanol	176		47	62	60
2-Octanol	179		32	63	114
1,2-Propanediol	187		—	153 (di)	—
1-Octanol	194		61	67	74
1,2-Ethandiol	197		169 (di)	176 (di)	157 (di)
1-Phenylethanol	202	20	93	106	92
Benzyl alcohol	205		112	134	77
1,3-Propanediol	214		178 (di)	164 (di)	137 (di)
2-Phenylethanol	219		108	119	78
1-Decanol	231		57	73	59
3-Phenyl-1-propanol	236		92	—	45
Cinnamyl alcohol	257	33	121	114	90
1-Dodecanol (lauryl alcohol)	259	24	60	80	74
4-Methoxybenzyl alcohol	259	24	—	—	92
Glycerol	290d		—	191 (tri)	180 (tri)
(-)-Menthol		43	153	119	111

TABLE 1 Alcohols (continued)

Compound	bp, °C	mp, °C	3,5-Dinitrobenzoate	1-Naphthylurethane	Phenylurethane
2,2-Dimethyl-1-propanol	113	53	—	100	144
Diphenylmethanol (benzhydrol)	288	69	141	135	139
Benzoin		133 (137)	—	140	165
(-)-Cholesterol		148	—	176	168
(-)-Borneol		208	154	132	138

TABLE 2 Aldehydes

Compound	bp, °C	mp, °C	2,4-Dinitrophenylhydrazone	Semicarbazone
Propanal	49		150	89 (154)
2-Butenal (trans)	103		190	199
Hexanal	128		104	106
Heptanal	155		108	109
2-Furancarboxaldehyde	161		229 (212)	202
Cyclohexane-carboxaldehyde	161		172	173
Octanal	171		106	98
Benzaldehyde	179		237	222
Phenylethanal	194	34	121	153
2-Hydroxybenzaldehyde	196		248	231
4-Methylbenzaldehyde	204		232	234 (215)
2-Chlorobenzaldehyde	213		212	225 (146)
3-Phenylpropanal	224		149	127
3-Bromobenzaldehyde	235		—	205
2-Methoxybenzaldehyde	245	38	253	215d
4-Methoxybenzaldehyde	247		254	210
Cinnamaldehyde (trans)	252		255d	215
3,4-Methylenedioxybenzaldehyde	263	37	266d	230
3,4-Dimethoxybenzaldehyde		44	262	177
4-Chlorobenzaldehyde	214	47	254	230
4-Bromobenzaldehyde		56	257	228
3-Nitrobenzaldehyde		58	293d	246
4-Hydroxy-3-methoxybenzaldehyde (Vanillin)		80	271d	229
3-Hydroxybenzaldehyde		104	257d	198
4-Hydroxybenzaldehyde		115	280d	224

TABLE 3 Amines

Compound	Class ^a	bp, °C	mp, °C	Benzamide ^b	Benzenesulfonamide ^b	Picrate ^b
<i>tert</i> -Butylamine	1°	46		134	—	198
Propylamine	1°	49		84	36	135
Diethylamine	2°	55		42	42	155
Allylamine	1°	58		—	39	140
<i>sec</i> -Butylamine	1°	63		76	70	139
2-Amino-2-methylbutane	1°	77		—	—	183
Butylamine	1°	77		42	—	151
Diisopropylamine	2°	83		—	—	140
Pyrrolidine	2°	89		—	—	112 (163)
Triethylamine	3°	89		—	—	173
1-Aminopentane	1°	104		—	—	139
Piperidine	2°	105		48	93	152
Dipropylamine	2°	110		—	51	75
Ethylenediamine	1°	116		244 (di)	168 (di)	233 (di)
1-Aminohexane	1°	129		40	96	126
Morpholine	2°	130		75	118	146
Diisobutylamine	2°	138		—	55	121
2-Aminoheptane	1°	143		—	—	—
1-Aminoheptane	1°	155		—	—	121
Tripropylamine	3°	156		—	—	116
Dibutylamine	2°	160		—	—	59
1-Amino-2-propanol	1°	163		—	—	142
Indole-3-acetic acid	2°	168		—	—	—
2-Fluoroaniline	1°	176		113	—	—
<i>N,N</i> -Dimethylbenzylamine	3°	182		—	—	93
<i>N</i> -Methylbenzylamine	2°	182		—	—	117
Benzylamine	1°	184		105	88	194
4-Fluoroaniline	1°	186		185	—	—
1-Phenylethylamine	1°	187		120	—	—
2-Phenylethylamine	1°	198		116	69	174
Tributylamine	3°	216		—	—	106
4-Aminomethylpyridine	1° (3°)	230		—	—	—
Aminodiphenylmethane	1°	295		—	—	—
2-Amino-6-methylpyridine	1° (3°)	208	41	90	—	202
2-Benzoylpyridine	3°		42	—	—	130
4-Methylaniline	1°	200	45	158	120	182
2-Aminobiphenyl	1°		49	102	—	—
6-Amino-1-hexanol	1°		57	—	—	—
Methoxyaniline	1°		58	154	95	—
4-Bromoaniline	1°	245d	66	204	134	180
4-Iodoaniline	1°		67	222	—	—
2-Nitroaniline	1°		71	110	104	73
4-Chloroaniline	1°		72	192	122	—
Tribenzylamine	3°		91	—	—	190
3-Nitroaniline	1°		113	155	136	143
2,4,6-Tribromoaniline	1°		119	198	—	—
3-Aminophenol	1°		122	174 (198)	—	—
3-(Dimethylaminomethyl)-indole	3°		133	—	—	—
2-Aminobenzoic acid	1°		146	182	—	104
4-Nitroaniline	1°		147	199	139	100

TABLE 3 Amines (continued)

Compound	Class ^a	bp, °C	mp, °C	Benzamide ^b	Benzenesulfonamide ^b	Picrate ^b
3-Aminobenzoic acid	1°		173	248	—	—
2-Aminophenol	1°		174	—	141	—
4-Aminophenol	1°		184	234 (di)	125	—
4-Aminobenzoic acid	1°		189	278	—	—
β-Alanine	1°		200d	120	—	—
Glycine	1°		230d	188	—	202

a. 1°, primary; 2°, secondary; 3°, tertiary.

b. Procedures for preparation of derivatives can be found in Ref. 1.

TABLE 4 Carboxylic acids

Compound	bp, °C	mp, °C	MW	Amide	Anilide
Formic acid	100		46	—	50
Acetic acid	118		60	82	114
Propanoic acid	140		74	81	105
Chloroacetic acid	185	61	94	121	135
2-Chloropropanoic acid	186		108	80	92
Dichloroacetic acid	194		128	98	118
2-Bromopropanoic acid	204	24	153	123	99
Bromoacetic acid	208	50	139	91	131
Octanoic acid	236		144	110	57
Decanoic acid	270	30	172	108 (100)	70
3-Chloropropanoic acid		41	107	101	—
Dodecanoic acid (lauric acid)		43	200	99	78
3-Phenylpropanoic acid	280	48 (40)	110	82 (105)	96
Trichloroacetic acid		57	163	141	97
2-Butenoic acid (trans)		72	86	160	118
Phenylacetic acid		76	136	156	117
2-Benzoylbenzoic acid (monohydrate)		90	208	165	195
		(anhydrous, 128)	226		
Pentanedioic acid (glutaric acid)		97	132	175 (di)	224 (di)
Phenoxyacetic acid		99	152	101	99
2-Methoxybenzoic acid		100	152	129	—
Citric acid (monohydrate)		100	210	210 (tri)	192 (tri)
		(anhydrous, 153)	192		
Oxalic acid (dihydrate)		104	126	419d (di)	254 (di)
4-Chlorophenylacetic acid		105	170	175	164
2-Methylbenzoic acid		105	136	142	125
3-Methylbenzoic acid		111	136	94	126
(1)- or (2)-Mandelic acid		118	152	133	151
3-Furancarboxylic acid		121	112	169	—
Benzoic acid		122	122	130	160
Maleic acid		130	116	260 (181) (di)	187 (di)
Cinnamic acid (trans)		133	148	147	153 (109)
2-Furancarboxylic acid		134	112	143	123
Decanedioic acid (sebacic acid)		134	202	210 (di)	202 (di)

TABLE 4 Carboxylic acids (continued)

Compound	bp, °C	mp, °C	MW	Amide	Anilide
Acetylsalicylic acid		136	180	138	136
2-Chlorobenzoic acid		140	156	142 (202)	114
3-Nitrobenzoic acid		140	167	142	153
2-Nitrobenzoic acid		146	167	174	155
2-Aminobenzoic acid		146	136	109	131
Diphenylacetic acid		148	212	168	180
Benzilic acid		150	228	153	174
2-Bromobenzoic acid		150	201	155	141
Hexanedioic acid (adipic acid)		153	146	220 (di)	240 (di)
3-Chlorobenzoic acid		158	156	134	122
2-Hydroxybenzoic acid (salicylic acid)		159	138	139	136
1-Naphthoic acid		160	172	203	163
2-Iodobenzoic acid		162	248	110	141
2,4-Dichlorobenzoic acid		162	191	194	—
(1)-Tartaric acid		169	150	195 (di)	263 (di)
4-Methylbenzoic acid		180	136	160	145
3,4-Dimethoxybenzoic acid		182	182	164	154
4-Methoxybenzoic acid		184	152	167	169
Butandioic acid (succinic acid)		185	118	260 (di)	230 (di)
4-Aminobenzoic acid		189	136	—	—
Hippuric acid (<i>N</i> -benzoylglycine)		190	179	183	208
β -Alanine		200d	89	—	—
Phthalic acid		206d	166	220 (di)	253 (di)
4-Hydroxybenzoic acid		215	138	162	196
Glycine		230d	75	—	—
4-Nitrobenzoic acid		241	167	201	211
4-Chlorobenzoic acid		242	156	179	194
Fumaric acid		286	116	266 (di)	313 (di)

TABLE 5 Esters

Compound	bp, °C	mp, °C
Ethyl formate	54	
Methyl acetate	57	
Ethyl trifluoroacetate	61	
Ethyl acetate	77	
<i>tert</i> -Butyl acetate	98	
Propyl acetate	101	
Allyl acetate	103	
1-Methylpropyl acetate	112	
2-Methyl-1-propyl acetate	117	
Methyl 2-butenate (<i>trans</i>)	119	
1-Butyl acetate	126	
3-Methyl-1-butyl acetate	142	
1-Butyl propanoate	146	
1-Pentyl acetate	149	
Ethyl 2-oxopropanoate	155	

TABLE 5 Esters (continued)

Compound	bp, °C	mp, °C
Ethyl hexanoate	168	
Ethyl trichloroacetate	168	
Methyl acetoacetate	170	
2-Furylmethyl acetate	176	
Ethyl acetoacetate	181	
Methyl 2-furoate	181	
Dimethyl butanedioate	196	
Phenyl acetate	197	
Methyl benzoate	199	
4-Hydroxybutanoic acid lactone	204	
Ethyl 4-oxopentanoate	206	
4-Hydroxypentanoic acid lactone	207	
Ethyl benzoate	213	
Benzyl acetate	216	
Diethyl butanedioate	217	
Diethyl (<i>E</i>)-2-butenedioate	218	
Diethyl (<i>Z</i>)-2-butenedioate	222	
Methyl 2-hydroxybenzoate	223	
(-)-Bornyl acetate	223	29
Ethyl 2-hydroxybenzoate	234	
1-Butyl 4-oxopentanoate	237	
Ethyl decanoate	244	
1-Butyl benzoate	250	
Glyceryl triacetate	258	
Ethyl benzoylacetate	265	
Ethyl dodecanoate	269	
Ethyl cinnamate (<i>trans</i>)	271	
Dimethyl phthalate	284	
Dibutyl phthalate	340	
Benzyl benzoate	323	21
Methyl 3-pyridinecarboxylate	209	42
Phenyl 2-hydroxybenzoate		42
1-Naphthyl acetate		48
Methyl 2-hydroxy-2-phenylacetate		52
Phenyl benzoate		70
Diphenyl phthalate		75
Cholesteryl acetate		116 (94)
Ethyl 4-hydroxybenzoate		116
Acetylsalicylic acid (Aspirin)		136

TABLE 6 Ketones

Compound	bp, °C	mp, °C	2,4-Dinitrophenyl hydrazone	Semicarbazone
Acetone	56		126	190
2-Butanone	80		117	136
2,3-Butanedione	88		314 (di)	278 (di) 235 (mono)
3-Methyl-2-butanone	94		120	113
2-Pentanone	102		144	110
3-Pentanone	102		156	139
3,3-Dimethyl-2-butanone (pinacolone)	106		125	157
4-Methyl-2-pentanone	116		95	133
2,4-Dimethyl-3-pentanone	125		95	160
3-Hexanone	125		130	113
2-Hexanone	129		106 (110)	12
Cyclopentanone	131		146	210
2,4-Pentanedione	139		209 (di)	209 (di) 122 (mono)
4-Heptanone	144		75	133
3-Hydroxy-2-butanone (acetoin)	145		318	185 (202)
3-Heptanone	148		—	103 (152)
2-Heptanone	151		89	127
Ethyl 2-oxopropanoate	155		—	—
Cyclohexanone	156		162	166
4-Hydroxy-4-methyl-2-pentanone	166		203	—
3-Octanone	167		—	—
2,6-Dimethyl-4-heptanone	168		66 (92)	126
3-Methylcyclohexanone	169		155	179 (191)
Methyl acetoacetate	170		—	152
4-Methylcyclohexanone	171		134	199
2-Octanone	172		58	122
Ethyl acetoacetate	181		93	133
Cycloheptanone	181		148	163
5-Nonanone	187		—	90
2,5-Hexanedione	194		257 (di)	224 (di) 185 (mono)
2,6-Dimethyl-2,5-heptadien-4-one (phorone)	198	27	118	221 (186)
Acetophenone	204	20	240 (250)	198
Ethyl 4-oxopentanoate	206		102	148
1-Phenyl-2-propanone	216	27	156	199
Propiophenone	218	20	191	174
2-Methyl-1-phenyl-1-propanone	222		163	181
1-Phenyl-2-butanone	226		—	135 (146)
4-Methylacetophenone	226	28	260	205
(-)-Carvone	230		191	162
4-Chloroacetophenone	232		231	204 (160)
Butyl 4-oxopentanoate	237		—	—
4-Methoxyacetophenone	258	37	220 (231)	197
Ethyl benzoylacetate	265		—	125
1-Acetylnaphthalene	302		—	289 (233)
1,3-Diphenylacetone	330	33	100	146 (126)
2-Benzoylpyridine		42	199	—
Benzoin methyl ether		48	—	—

TABLE 6 Ketones (continued)

Compound	bp, °C	mp, °C	2,4-Dinitrophenyl hydrazone	Semicarbazone
Benzophenone		48	239 (229)	164
4-Bromoacetophenone		51	230 (237)	208
2-Acetylnaphthalene		53	262	235
1,3-Diphenyl-2-propen-1-one (benzalacetophenone)		58	244	170 (179)
Benzoin ethyl ether		60	—	—
4-Methoxybenzophenone		62	180	—
4-Nitroacetophenone		80	—	—
3-Nitroacetophenone		81	228	257
Fluorenone		83	283	234
Benzil		95	189 (di)	244 (di) 174 (mono)
2-Benzoylbenzoic acid		128	—	—
Benzoin		133 (137)	245	206
4-Hydroxybenzophenone		134	242	194
(±)-Camphor		174	164	247 (237)
(+)-Camphor		180	177	—
Ninhydrin		243	—	—

TABLE 7 Phenols

Compound	bp, °C	mp, °C	Bromo derivative	1-Naphthyl- urethane	3,5-Dinitro- benzoate
2-Hydroxybenzaldehyde	196		—	—	—
2-Methoxyphenol (guaiacol)	205	32	116 (tri)	118	141
4-Chlorophenol	217	37 (43)	90 (di)	166	186
Methyl 2-hydroxybenzoate	223		—	—	—
2-tert-Butylphenol	224		—	—	—
Ethyl 2-hydroxybenzoate	234		—	—	—
Phenyl 2-hydroxybenzoate		42	—	—	—
2-Nitrophenol		45	117 (di)	113	155
5-Methyl-2-isopropyl- phenol (thymol)		50	55 (mono)	160	103
4-Hydroxy-3-methoxy- benzaldehyde (vanillin)		80	160	—	—
1-Naphthol		94	105 (di)	152	217
4-tert-Butylphenol		100	65 (di)	110	—
3-Hydroxybenzaldehyde		104	—	—	—
1,2-Dihydroxybenzene (catechol)		106	192 (tetra)	175	152 (di)
1,3-Dihydroxybenzene (resorcinol)		110	112 (di)	206	201 (di)
2-Chloro-4-nitrophenol		111	—	—	—
4-Nitrophenol		114	142 (di)	151	186
4-Hydroxybenzaldehyde		116	181 (di)	—	—
Ethyl 4-hydroxybenzoate		116	—	—	—

TABLE 7 Phenols (continued)

Compound	bp, °C	mp, °C	Bromo derivative	1-Naphthyl-urethane	3,5-Dinitrobenzoate
1,3,5-Trihydroxybenzene (phloroglucinol)		117 (dihyd) 219 (anhy)	151 (tri)	—	—
3-Aminophenol	122		—	—	179
2-Naphthol	123		84	156	210
1,2,3-Trihydroxybenzene (pyrogallol)	133		158 (di)	—	205 (tri)
4-Hydroxybenzophenone	134		—	—	—
2-Hydroxybenzanilide	136		—	—	—
2-Hydroxybenzamide	141		—	—	—
2-Hydroxybenzoic acid (salicylic acid)	159		—	—	—
4-Acetamidophenol	169		—	—	—
1,4-Dihydroxybenzene (hydroquinone)	171		186 (di)	—	317 (di)
2-Aminophenol	174		—	—	—
4-Aminophenol	184		—	—	178
4-Hydroxybenzoic acid	215		—	—	—
Phenolphthalein	265		—	—	—