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Thermodynamic properties of organic compounds: enthalpy of fusion and melting point temperature compilation

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Abstract

Published enthalpies of fusion and melting point temperatures have been gathered from the chemical literature and are presented in tabular form according to increasing carbon and hydrogen atom numbers. References are also provided to indicate the literature sources consulted.

INTRODUCTION

Aqueous solubility data of organic compounds are becoming increasingly important, particularly in the light of known carcinogenic/mutagenic activity of select classes of aromatic compounds and the frequent danger imposed by pollution of natural waterways by petroleum and toxic wastes. Data for a number of polycyclic aromatic hydrocarbons (PAHs), heterocyclic polynuclear aromatics, halogenated benzenes, polychlorinated biphenyls (PCBs) and polychlorinated dibenzodioxins (PCDDs) have been published in recent chemical literature. Despite efforts by experimentalists and scientific organizations, both in terms of new experimental measurements and critically evaluated data compilations, there are numerous common organic pollutants for which actual solubility data are still not readily available.

To address this problem, researchers have turned to predictive methods as a means to generate desired quantities. Numerous linear and multilinear regression equations have been derived expressing the logarithm of the aqueous mole fraction solubility (or molar solubility) as a function of empirically derived quantities such as van der Waals volumes, total molecular and group surface areas, molecular weight, and a variety of other molecular connectivity and topological indices. For non-polar solutes, molecular size descriptors provide a very rough measure of the energy required to create a solvent cavity wherein a solute molecule would reside. As water is a highly structured solvent, the number of hydrogen bonds that must be broken is directly proportional to the size of the dissolved solute. Secondary considerations involve the energetics of breaking solute–solute

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TABLE 1
Molar enthalpies of fusion (J mol^{-1}) and melting point temperatures (°C)

Formula	Chemical name	T_{mp}	$\Delta \bar{H}^{fus}$	Ref.
$CBrCl_3$	Bromotrichloromethane	−5.7	2540	5
CCl_2O	Phosgene	−127.9	5740	5
CCl_3NO_2	Chloropicrin	−64.0	33120	5
CCl_4	Tetrachloromethane	−23.0	3275	5
CS_2	Carbon disulfide	−111.5	4395	5
$CHCl_3$	Trichloromethane	−63.6	8800	5
CHN	Hydrogen cyanide	−13.4	8410	5
CH_2N_2	Cyanamide	44.0	8760	5
CH_2O_2	Formic acid	8.3	12720	5
CH_3Br	Bromomethane	−93.7	5980	5
CH_4	Methane	−182.5	936	5
CH_3D	Monodeuteromethane	−182.7	910	5
CD_4	Deuteromethane	−183.4	900	5
CH_4N_2S	Thiourea	172.4	14420	6
CH_4O	Methanol	−97.9	3180	5
CH_4S	Methyl mercaptan	−121.0	5900	5
CH_5N	Methylamine	−93.5	6130	5
$C_2Br_2F_4$	1,2-Dibromotetrafluoroethane	−110.4	7040	7
$C_2Cl_2F_4$	1,2-Dichlorotetrafluoroethane	−92.6	1510	8
$C_2Cl_3F_3$	1,1,2-Trichlorotrifluoroethane	−36.2	2470	8
$C_2Cl_4F_2$	1,1,2,2-Tetrachlorodifluoroethane	26.5	3700	8, 9
$C_2HCl_3O_2$	Trichloroacetic acid	57.5	5880	5
$C_2H_2Br_2Cl_2$	1,2-Dibromo-1,1-dichloroethane	−66.9	8300	5
$C_2H_2Cl_2O_2$	Dichloroacetic acid	10.8	7665	5
$C_2H_3Br_3$	1,1,2-Tribromoethane	−29.2	9110	5
$C_2H_3ClO_2$	α-Trichloroacetic acid	61.2	12280	5
$C_2H_3ClO_2$	β-Trichloroacetic acid	56.0	13885	5
$C_2H_3Cl_3$	1,1,1-Trichloroethane	−30.4	2730	5
$C_2H_3Cl_3$	1,1,2-Trichloroethane	−36.6	11540	5
$C_2H_3F_3$	1,1,1-Trifluoroethane	−111.3	6190	5
$C_2H_4Br_2$	1,2-Dibromoethane	9.9	10840	5
$C_2H_4Cl_2$	1,2-Dichloroethane	−35.5	8830	5
$C_2H_4N_4$	1*H*-1,2,4-triazol-3-amine	155.1	21930	6
C_2H_5Cl	Chloroethane	−138.3	4450	5
C_2H_6	Ethane	−183.3	2860	5
$C_2H_6N_2O$	Methylurea	100.6	15750	10
C_2H_6O	Dimethyl ether	−141.5	4940	5
C_2H_6O	Ethanol	−114.5	5020	5
$C_2H_6O_2$	Ethylene glycol	−11.5	11230	5
C_2H_6S	Dimethyl sulfide	−98.3	7990	5
C_2H_6S	Ethanethiol	−121.0	4975	5
$C_2H_6S_2$	Methyl disulfide	−120.5	9190	5
C_2H_7N	Dimethylamine	−92.2	5940	5
$C_2H_8N_2$	Ethylenediamine	11.1	22580	11
$C_3H_2Cl_3F_3$	1,1,1-Trichloro-3,3,3-trifluoropropane	−40.5	14070	12
C_3H_3N	Acrylonitrile	−83.5	6230	13
$C_3H_3N_3$	1,3,5-Triazine	80.2	14560	14
$C_3H_4O_2$	Acrylic acid	12.3	11160	5

TABLE 1 (continued)

Formula	Chemical name	T_{mp}	$\Delta \overline{H}^{fus}$	Ref.
$C_3H_5Br_3$	1,2,3-Tribromopropane	16.2	23780	5
$C_3H_5N_3O_9$	Trinitroglycerol	12.3	21870	5
C_3H_6	Cyclopropane	−127.4	5445	5
C_3H_6	Propene	−185.3	3000	5, 15
$C_3H_6Br_2$	1,3-Dibromopropane	−34.2	13600	5
$C_3H_6Cl_2$	1,2-Dichloropropane	−100.5	6400	5
C_3H_6O	Acetone	−94.8	5690	5
$C_3H_6O_3$	1,3,5-Trioxane	60.2	15100	14
$C_3H_6O_3S$	1,3-Propane sulfone	29.1	9960	6
C_3H_7Cl	2-Chloropropane	−117.2	7390	5
C_3H_7N	Cyclopropylamine	−35.4	13180	16
$C_3H_7NO_2$	Ethyl carbamate	48.7	15230	5
C_3H_8	Propane	−181.7	3530	5
$C_3H_8N_2O$	Ethylurea	94.6	13940	10
$C_3H_8N_2O$	1,1-Dimethylurea	180.8	29610	10
$C_3H_8N_2O$	1,3-Dimethylurea	106.3	13620	10
C_3H_8O	1-Propanol	−126.1	5195	5
C_3H_8O	2-Propanol	−89.5	5375	5
$C_3H_8O_3$	Glycerol	18.2	8475	5
C_3H_9N	Trimethylamine	−117.1	6550	5
C_3H_9N	1-Aminopropane	−84.8	10970	13
C_3H_9N	2-Aminopropane	−95.2	7325	13
$C_4H_4N_2$	Succinonitrile	54.5	3920	5
$C_4H_4O_3$	Succinic anhydride	119.0	20410	5
C_4H_4S	Thiophene	−39.4	4970	5
C_4H_5N	Pyrrole	−23.4	7910	17
C_4H_6	1,3-Butadiene	−108.9	7980	5
C_4H_6	2-Butyne	−32.4	9230	5
$C_4H_6O_2$	Crotonic acid	72.0	9120	5
$C_4H_6O_2$	*cis*-Crotonic acid	71.2	12570	5
$C_4H_6O_2$	γ-Butyrolactone	−43.4	9570	18
$C_4H_6O_4$	Dimethyl oxalate	54.4	21,070	5
$C_4H_6O_4$	Succinic acid	183.8	32950	19
C_4H_8	Isobutene	−140.4	5930	5
C_4H_8	*cis*-2-Butene	-138.9	7580	5, 15
$C_4H_8N_2S$	Allyl thiourea	77.0	16260	5
C_4H_8O	Tetrahydrofuran	−108.4	8540	20
C_4H_8O	2-Butanone	−86.7	8440	21
$C_4H_8O_2$	Ethyl acetate	−83.6	10480	5
$C_4H_8O_2$	*n*-Butyric acid	−5.7	11080	5
$C_4H_8O_2$	*p*-Dioxane	11.0	12850	5
C_4H_9Br	2-Bromobutane	−112.7	6880	5
C_4H_{10}	Butane	−138.3	4660	5
C_4H_{10}	Isobutane	−159.4	4610	5
$C_4H_{10}N_2O$	Propylurea	107.8	14630	10
$C_4H_{10}N_2O$	Isopropylurea	154.2	17400	10
$C_4H_{10}N_2O$	1,1,3-Trimethylurea	71.2	14300	10
$C_4H_{10}O$	1-Butanol	−89.8	9280	5
$C_4H_{10}O$	*tert*-Butanol	25.4	6790	5

TABLE 1 (continued)

Formula	Chemical name	T_{mp}	$\Delta \bar{H}^{fus}$	Ref.
$C_4H_{10}O$	Ethyl ether	−116.3	7270	5
$C_4H_{12}ClN$	2-Aminobutane hydrochloride	148.1	10060	6
$C_4H_{12}Si$	Tetramethylsilane	−99.0	6880	5
$C_5H_6N_2$	4-Aminopyridine	156.8	20065	6
C_5H_8	Cyclopentene	−135.1	3360	5
C_5H_8	Isoprene	−145.9	4790	5
C_5H_8	Methylcyclobutane	−134.6	5760	16, 22
C_5H_8	1,4-Pentadiene	−148.8	6140	5
$C_5H_8O_2$	δ-Valerlactone	−10.3	10530	18
$C_5H_8O_3$	Levulinic acid	33.0	9220	5
$C_5H_8O_4$	Glutaric acid	97.8	20900	19
C_5H_{10}	1-Pentene	−166.2	5810	5, 15
C_5H_{10}	*cis*-2-Pentene	−151.4	7110	5, 15
C_5H_{10}	*trans*-2-Pentene	−140.2	8360	5, 15
C_5H_{10}	Cyclopentane	−93.8	610	5
$C_5H_{10}N_2O_2S$	5-Methyl-*N*-(methylcarbamoyloxy)thio-acetimidate	79.5	21730	6
$C_5H_{10}O$	2-Pentanone	−76.9	10630	23
$C_5H_{10}O$	3-Pentanone	−39.0	11590	23
$C_5H_{10}S$	Tetrahydrothiopyran	18.4	2360	24
$C_5H_{11}N$	Cyclopentylamine	−82.7	8310	16
C_5H_{12}	Pentane	−129.7	8420	5
C_5H_{12}	Isopentane	−159.9	5150	5
C_5H_{12}	2,2-Dimethylpropane	−16.6	3260	5
$C_5H_{12}NO_3PS$	*O*,*O*-Dimethyl-(*S*-methylcarbamoyl-methyl)phosphorodithioate	48.1	20490	6
$C_5H_{12}N_2O$	1,3-Diethylurea	110.2	12460	10
$C_5H_{12}N_2O$	1,1-Diethylurea	69.1	16780	10
$C_5H_{12}N_2O$	Butylurea	96.1	14550	10
$C_5H_{12}N_2O$	*tert*-Butylurea	176.6	33130	10
$C_5H_{12}O$	1-Pentanol	−78.9	9380	5
$C_6Cl_3F_3$	1,3,5-Trichloro-2,4,6-trifluorobenzene	61.8	19830	25, 26
$C_6Cl_4O_2$	2,3,5,6-Tetrachloro-2,5-cyclohexadiene-1,4-dione	294.0	30870	6
$C_6Cl_5NO_2$	Pentachloronitrobenzene	144.8	18410	6, 27
C_6Cl_6	Hexachlorobenzene	231.8	23850	6, 28, 29
$C_6F_5NO_2$	Pentafluoronitrobenzene	−22.7	11810	30
$C_6HCl_4NO_2$	1,2,4,5-Tetrachloro-3-nitrobenzene	100.1	19460	6
C_6HCl_5	Pentachlorobenzene	84.5	20600	29
C_6HCl_5O	Pentachlorophenol	189.3	17150	6, 28
C_6HF_5	Pentafluorobenzene	−47.3	10850	31
C_6HF_5O	Pentafluorophenol	32.8	12840	32
$C_6H_2Cl_4$	1,2,3,4-Tetrachlorobenzene	46.8	17000	29
$C_6H_2Cl_4$	1,2,4,5-Tetrachlorobenzene	148.0	24100	29
$C_6H_2Cl_4$	1,2,3,5-Tetrachlorobenzene	50.7	19000	29
$C_6H_2Cl_5N$	Pentachloroaniline	232.6	18700	6
$C_6H_3BrCl_2O$	4-Bromo-2,5-dichlorophenol	70.2	22110	6
$C_6H_3Br_3O$	2,4,6-Tribromophenol	93.0	18520	5
$C_6H_3Cl_3$	1,2,3-Trichlorobenzene	53.7	20500	6, 28, 29

TABLE 1 (continued)

Formula	Chemical name	T_{mp}	$\Delta\overline{H}^{fus}$	Ref.
$C_6H_3Cl_3$	1,3,5-Trichlorobenzene	63.5	18200	6, 28, 29
$C_6H_3Cl_3O$	2,4,5-Trichlorophenol	68.5	23850	6, 27
$C_6H_3Cl_4N$	2-Chloro-6-(trichloromethyl)pyridine	64.6	19480	6
C_6H_4BrI	*o*-Bromoiodobenzene	21.0	14420	5
C_6H_4BrI	*m*-Bromoiodobenzene	9.3	12160	5
C_6H_4BrI	*p*-Bromoiodobenzene	90.1	19130	5
$C_6H_4Br_2$	*o*-Dibromobenzene	1.8	12610	5
$C_6H_4Br_2$	*m*-Dibromobenzene	−6.9	13210	5
$C_6H_4Br_2$	*p*-Dibromobenzene	86.0	20280	5
$C_6H_4Br_2O$	2,4-Dibromophenol	12.0	14720	5
$C_6H_4ClNO_2$	*m*-Chloronitrobenzene	44.4	19370	5
$C_6H_4ClNO_2$	*p*-Chloronitrobenzene	83.5	20780	5
$C_6H_4Cl_2$	*o*-Dichlorobenzene	−16.7	12930	5, 6
$C_6H_4Cl_2$	*m*-Dichlorobenzene	−24.8	12640	5
$C_6H_4Cl_2$	*p*-Dichlorobenzene	52.7	17150	5, 6, 28
$C_6H_4Cl_2N_2O_2$	2,6-Dichloro-4-nitroaniline	193.6	32640	6, 28
$C_6H_4Cl_2O$	2,3-Dichlorophenol	56.8	21360	33
$C_6H_4Cl_2O$	2,4-Dichlorophenol	44.8	20090	33
$C_6H_4Cl_2O$	2,5-Dichlorophenol	57.8	22430	33
$C_6H_4Cl_2O$	2,6-Dichlorophenol	66.8	22140	33
$C_6H_4Cl_2O$	3,4-Dichlorophenol	67.8	20930	6, 33
$C_6H_4Cl_2O$	3,5-Dichlorophenol	67.8	20510	33
$C_6H_4I_2$	*o*-Diiodobenzene	23.4	14010	5
$C_6H_4I_2$	*m*-Diiodobenzene	34.2	15930	5
$C_6H_4I_2$	*p*-Diiodobenzene	129.0	22360	5
$C_6H_4N_2O_4$	*o*-Dinitrobenzene	116.9	22680	5
$C_6H_4N_2O_4$	*m*-Dinitrobenzene	89.7	17370	5
$C_6H_4N_2O_4$	*p*-Dinitrobenzene	173.5	28130	5
$C_6H_4N_2O_5$	2,3-Dinitrophenol	143.8	26240	33
$C_6H_4N_2O_5$	2,4-Dinitrophenol	114.8	24170	33
$C_6H_4N_2O_5$	2,5-Dinitrophenol	107.8	23730	33
$C_6H_4N_2O_5$	2,6-Dinitrophenol	62.8	19580	33
$C_6H_4N_2O_5$	3,4-Dinitrophenol	133.8	25370	33
$C_6H_4O_2$	*p*-Benzoquinone	112.9	18530	5
C_6H_5Br	Bromobenzene	−30.6	10620	5
C_6H_5BrO	4-Bromophenol	63.5	14840	5
C_6H_5Cl	Chlorobenzene	−45.2	9610	5
C_6H_5ClO	2-Chlorophenol	9.8	12520	33
C_6H_5ClO	3-Chlorophenol	32.6	14910	33
C_6H_5ClO	4-Chlorophenol	42.7	14070	33
C_6H_5F	Fluorobenzene	−42.2	11310	34
C_6H_5I	Iodobenzene	−31.3	9760	5
$C_6H_5NO_2$	Nitrobenzene	5.7	11590	5
$C_6H_5NO_3$	2-Nitrophenol	44.8	17440	5, 33
$C_6H_5NO_3$	3-Nitrophenol	96.8	19200	33
$C_6H_5NO_3$	4-Nitrophenol	113.8	18250	5, 6, 33
C_6H_6	Benzene	5.5	9950	5
$C_6H_6Cl_6$	1α,2α,3β,4α,5α,6β-Hexachloro-cyclohexane	113.6	22130	6

TABLE 1 (continued)

Formula	Chemical name	T_{mp}	$\Delta \overline{H}^{fus}$	Ref.
$C_6H_6N_2O_2$	*o*-Nitroaniline	71.2	16110	5
$C_6H_6N_2O_2$	*m*-Nitroaniline	114.0	23680	5
$C_6H_6N_2O_2$	*p*-Nitroaniline	147.0	21090	5
C_6H_6O	Phenol	40.9	11290	5
$C_6H_6O_2$	1,2-Dihydroxybenzene	105.0	22760	5, 6
$C_6H_6O_2$	1,3-Dihydroxybenzene	110.0	21290	5
$C_6H_6O_2$	1,4-Dihydroxybenzene	172.3	27110	5
C_6H_6S	Thiophenol	−14.9	11480	5
C_6H_7N	Aniline	−6.3	10560	5
$C_6H_8N_2$	Phenylhydrazine	19.6	16430	5
$C_6H_8N_2$	*p*-Phenylenediamine	145.0	24860	35
$C_6H_8O_4$	Methyl fumarate	102.0	34930	5
C_6H_{10}	Cyclohexene	−103.5	3290	5
$C_6H_{10}O_4$	Adipic acid	153.2	34850	19
C_6H_{12}	Methylcyclopentane	−142.5	6930	5
C_6H_{12}	Cyclohexane	6.6	2630	5
C_6H_{12}	Tetramethylethylene	−74.6	5460	5
$C_6H_{12}O$	Cyclohexanol	24.5	1760	5
$C_6H_{12}O$	2-Hexanone	−55.5	14900	36
$C_6H_{12}O$	3-Hexanone	−55.5	13490	36
$C_6H_{12}O_2$	ϵ-Caprolactone	−1.0	13820	18
C_6H_{14}	2,2-Dimethylbutane	−99.0	580	5
C_6H_{14}	2,3-Dimethylbutane	−128.8	800	5
C_6H_{14}	*n*-Hexane	−95.3	13080	5
C_6H_{14}	2-Methylpentane	−153.7	6270	5
$C_6H_{14}O$	Isopropyl ether	−86.8	11030	5
$C_6H_{14}O$	*n*-Propyl ether	−126.1	8830	5
$C_6H_{14}O_2$	1,6-Hexanediol	41.5	22200	37
$C_6H_{14}O_2$	2,3-Dimethyl-2,3-butanediol	43.3	14650	38
C_7F_8	Octafluorotoluene	−65.6	11580	39
$C_7H_3Br_2NO$	3,5-Dibromo-4-hydroxybenzonitrile	190.8	32030	6
$C_7H_3Cl_2N$	2,6-Dichlorobenzonitrile	144.0	26170	6
$C_7H_3Cl_3O_2$	2,3,6-Trichlorobenzoic acid	129.5	23850	27
$C_7H_3F_5$	Pentafluorotoluene	−29.8	12990	40
$C_7H_3I_2NO$	4-Hydroxy-3,5-diiodobenzonitrile	209.8	33630	6
$C_7H_3I_3O_2$	2,3,5-Triiodobenzoic acid	230.6	32230	27
$C_7H_4Cl_2O_2$	3,5-Dichlorobenzoic acid	186.1	22970	6
$C_7H_4Cl_3NO_3$	3,5,6-Trichloro-2-pyridyloxyacetic acid	150.1	31170	6
$C_7H_5ClO_2$	2-Chlorobenzoic acid	140.2	25730	5
$C_7H_5ClO_2$	3-Chlorobenzoic acid	154.2	23840	5
$C_7H_5ClO_2$	4-Chlorobenzoic acid	239.7	32250	5
$C_7H_5Cl_2NO_2$	3-Amino-2,5-dichlorobenzoic acid	202.4	37420	6
$C_7H_5NO_4$	2-Nitrobenzoic acid	145.8	28010	5
$C_7H_5NO_4$	3-Nitrobenzoic acid	141.1	19290	5
$C_7H_5NO_4$	4-Nitrobenzoic acid	239.2	36920	5
$C_7H_5N_3O_6$	2,4,6-Trinitrotoluene	80.8	21230	5
$C_7H_6N_2O_4$	2,4-Dinitrotoluene	70.1	20120	5
$C_7H_6N_2O_5$	2-Methyl-4,6-dinitrophenol	86.1	19410	6
$C_7H_6O_2$	Benzoic acid	122.4	17310	5

TABLE 1 (continued)

Formula	Chemical name	T_{mp}	$\Delta \overline{H}^{fus}$	Ref.
$C_7H_6O_3$	4-Hydroxybenzoic acid	214.9	30900	5, 41
C_7H_7Br	4-Bromotoluene	28.0	14930	5
C_7H_7F	2-Fluorotoluene	−62.5	9800	42
C_7H_7F	3-Fluorotoluene	−89.2	8300	42
C_7H_7F	4-Fluorotoluene	−57.6	8800	42
C_7H_7NO	Benzamide	129.1	18490	43
$C_7H_7NO_2$	4-Nitrotoluene	51.6	16810	44
$C_7H_7NO_2$	2-Aminobenzoic acid	145.0	20640	5
$C_7H_7NO_2$	3-Aminobenzoic acid	179.5	21820	5
$C_7H_7NO_2$	4-Aminobenzoic acid	188.5	20920	5
$C_7H_7NO_3$	4-Nitro-5-methylphenol	127.8	27400	45
$C_7H_7NO_3$	2-Nitro-5-methylphenol	29.6	20790	46
C_7H_8	Toluene	−95.0	6850	5
C_7H_8	1,3,5-Cycloheptatriene	−75.2	1160	47
$C_7H_8N_2O$	Phenylurea	147.4	23680	48
C_7H_8O	Benzyl alcohol	−15.2	8970	5
C_7H_8O	2-Methylphenol	29.8	13940	42, 49
C_7H_8O	3-Methylphenol	11.8	9410	42, 49
C_7H_8O	4-Methylphenol	35.8	11890	5, 42, 49
C_7H_9N	*m*-Toluidine	−31.5	8800	42
C_7H_9N	*p*-Toluidine	43.3	17890	5, 42
C_7H_9N	*o*-Toluidine	−23.6	8100	42
C_7H_{12}	Cycloheptene	−56.2	970	50
$C_7H_{12}ClN_5$	6-Chloro-*N*, *N*-diethyl-1,3,5-triazine-2,4-diamine	229.3	47350	6
$C_7H_{12}O_4$	Pimilic acid	104.3	27620	19
C_7H_{14}	1-Heptene	−119.7	12660	5
C_7H_{14}	Methylcyclohexane	−126.6	6750	5
C_7H_{14}	Cycloheptane	−8.0	1880	47
$C_7H_{14}NO_5P$	Dimethyl(*E*)-1-methyl-2-methylcarbamolyvinyl phosphate	53.8	22360	6
C_7H_{16}	*n*-Heptane	−90.6	14160	5
C_7H_{16}	2-Methylhexane	−118.2	8870	5
C_7H_{16}	2,2-Dimethylpentane	−123.8	5860	5
C_7H_{16}	2,4-Dimethylpentane	−119.9	6690	5
C_7H_{16}	3,3-Dimethylpentane	−134.9	7070	5
C_7H_{16}	3-Ethylpentane	−118.6	9550	5
C_7H_{16}	2,2,3-Trimethylbutane	−25.0	2200	5
$C_7H_{16}O_2$	1,7-Heptanediol	22.0	21300	37
$C_8Cl_4N_2$	2,4,5,6-Tetrachloro-1,3-benzenedicarbonitrile	253.3	30000	6
$C_8H_4O_3$	Phthalic anhydride	130.1	23090	6
$C_8H_5Cl_3O_2$	2,3,6-Trichlorophenylacetic acid	159.1	22430	6
$C_8H_5Cl_3O_3$	(2,4,5-Trichlorophenoxy)acetic acid	155.6	38000	6
$C_8H_6Cl_2O_3$	3,6-Dichloro-2-methoxybenzoic acid	113.5	22900	6
$C_8H_6Cl_2O_3$	2,4-Dichloro-2-methoxybenzoic acid	139.3	35330	6
$C_8H_6Cl_2O_4$	3,6-Dichloro-5-hydroxy-2-methoxybenzoic acid	136.7	28980	6
$C_8H_6Cl_4$	Tetrachloro-*o*-xylene	86.0	21460	5

TABLE 1 (continued)

Formula	Chemical name	T_{mp}	$\Delta\bar{H}^{fus}$	Ref.
$C_8H_6Cl_4$	Tetrachloro-*p*-xylene	95.0	22590	5
$C_8H_6O_2$	Chromone	57.1	17310	51
$C_8H_7NO_2$	Methyl 4-aminobenzoate	111.9	22550	52
$C_8H_8Br_2$	α,α'-Dibromo-*o*-xylene	95.0	26780	5
$C_8H_8Br_2$	α,α'-Dibromo-*m*-xylene	77.0	23690	5
$C_8H_8Cl_2$	α,α'-Dichloro-*o*-xylene	55.0	21260	5
$C_8H_8Cl_2$	α,α'-Dichloro-*m*-xylene	34.0	19510	5
$C_8H_8Cl_2$	α,α'-Dichloro-*p*-xylene	100.0	23970	5
$C_8H_8Cl_2O_2$	1,4-Dichloro-2,5-dimethoxybenzene	130.7	27560	6
$C_8H_8O_2$	Phenylacetic acid	76.7	14490	5
$C_8H_8O_2$	*o*-Toluic acid	103.7	20170	5, 53
$C_8H_8O_2$	*m*-Toluic acid	108.8	15720	5
$C_8H_8O_2$	*p*-Toluic acid	179.6	22730	5
$C_8H_8O_3$	4-Hydroxyphenylacetic acid	150.4	28400	41
$C_8H_8O_3$	4-Methoxybenzoic acid	184.6	28400	41
$C_8H_8O_3$	Methyl 4-hydroxybenzoate	125.3	24310	54
$C_8H_9NO_2$	Methyl 4-aminobenzoate	111.2	24350	54
C_8H_{10}	*o*-Xylene	−25.2	13610	5
C_8H_{10}	*m*-Xylene	−47.8	11550	5
C_8H_{10}	*p*-Xylene	13.2	16805	5
$C_8H_{10}NO_5PS$	*O,O*-Dimethyl-*O*-4-nitrophenyl phosphorothioate	35.1	20070	6
$C_8H_{10}O$	2,3-Dimethylphenol	72.8	21020	33
$C_8H_{10}O$	2,5-Dimethylphenol	74.8	23380	33
$C_8H_{10}O$	2,6-Dimethylphenol	45.7	18900	33
$C_8H_{10}O$	3,4-Dimethylphenol	60.8	18130	33
$C_8H_{10}O$	3,5-Dimethylphenol	63.6	18000	33
C_8H_{12}	1,5-Cyclooctadiene	−69.2	9830	55
C_8H_{14}	Bicyclooctane	174.6	8350	56
$C_8H_{14}N_4OS$	4-Amino-6-(1,1-dimethylethyl)-3-(methylthio)-1,2,4-triazin-5(4*H*)-one	126.2	17995	6
$C_8H_{14}O_4$	Suberic acid	142.1	28820	19
C_8H_{16}	Cyclooctane	14.8	2410	47
C_8H_{16}	Ethylcyclohexane	−111.3	8330	5
C_8H_{16}	*trans*-1,1-Dimethylcyclohexane	−33.3	2060	5
C_8H_{16}	*cis*-1,2-Dimethylcyclohexane	−49.9	1640	5
C_8H_{16}	*trans*-1,2-Dimethylcyclohexane	−88.2	10490	5
C_8H_{16}	*cis*-1,3-Dimethylcyclohexane	−75.6	10820	5
C_8H_{16}	*trans*-1,3-Dimethylcyclohexane	−90.1	9860	5
C_8H_{16}	*cis*-1,4-Dimethylcyclohexane	−87.4	9310	5
C_8H_{16}	*trans*-1,4-Dimethylcyclohexane	−36.9	12330	5
$C_8H_{16}N_6$	1-(Methylamino)-3,5-bis(dimethylamino)-*s*-triazine	105.6	22340	57
$C_8H_{16}O_2$	Caprylic acid	16.3	21360	5, 58
C_8H_{18}	*n*-Octane	−56.8	20650	5
C_8H_{18}	3-Methylheptane	−120.5	11380	5
C_8H_{18}	4-Methylheptane	−121.0	10840	5
C_8H_{18}	2,2,4-Trimethylpentane	−107.3	9040	5
$C_8H_{18}N_2$	1,1-Dimethylazoethane	−14.6	10280	59

TABLE 1 (continued)

Formula	Chemical name	T_{mp}	$\Delta\overline{H}^{fus}$	Ref.
$C_8H_{18}N_2O$	1,1-Dimethylazoxyethane	15.2	11520	59
$C_8H_{18}O_2$	1,8-Octanediol	59.6	36100	37
$C_9H_4Cl_3NO_2S$	2[(Trichloromethyl)thio)]-1*H*-isoindole-1,3(2*H*)-dione	181.1	35490	6
C_9H_7N	Quinoline	−15.6	10800	5
$C_9H_8Cl_2O_3$	2-(2,4-Dichlorophenoxy)propanoic acid	116.1	30430	6
$C_9H_8Cl_2O_3$	Methyl 3,6-dichloro-2-methoxybenzoate	31.4	18490	6
$C_9H_8O_2$	Cinnamic acid	133.0	22630	5
$C_9H_8O_2$	Allocinnamic acid	68.0	16950	5
$C_9H_9ClO_3$	(4-Chloro-*o*-tolyloxy)acetic acid	119.7	29980	6
$C_9H_{10}BrClN_2O_2$	3-(4-Bromo-3-chlorophenyl)-1-methoxy-1-methylurea	96.6	26540	6
$C_9H_{10}O_2$	Hydrocinnamic acid	48.0	17680	5
$C_9H_{10}O_3$	4-Methoxyphenylacetic acid	84.9	21800	41
$C_9H_{10}O_3$	4-Hydroxyphenylpropionic acid	129.3	28900	41
$C_9H_{10}O_3$	4-Ethoxybenzoic acid	199.6	29400	41
$C_9H_{11}BrN_2O_2$	*N'*-(4-Bromophenyl)-*N*-methoxy-*N*-methylurea	95.1	24440	6
$C_9H_{11}ClN_2O$	3-(4-Chlorophenyl)-1,1-dimethylurea	174.4	29460	6
$C_9H_{11}Cl_3NO_3PS$	*O,O*-Diethyl-*O*-(3,5,6-trichloro-2-pyridyl) phosphorothioate	41.9	24530	6
$C_9H_{11}N$	5,6,7,8-Tetrahydroquinoline	−50.5	9075	60
$C_9H_{11}N$	1,2,3,4-Tetrahydroquinoline	16.8	11810	60
$C_9H_{11}NO_2$	Ethyl 4-aminobenzoate	89.6	23560	52, 54
C_9H_{12}	1,2,4-Trimethylbenzene	−43.8	3760	5
C_9H_{12}	1,2,3-Trimethylbenzene	−25.4	8370	5
C_9H_{12}	1,3,5-Trimethylbenzene	−44.7	9500	5
C_9H_{12}	*n*-Propylbenzene	−99.6	9270	61
$C_9H_{12}BrN_2O_2$	5-Bromo-6-methyl-3-(1-methylpropyl)-2,4-(1*H*, 3*H*)-pyrimidinedione	155.1	22020	6
$C_9H_{12}N_2O$	1,1-Dimethyl-3-phenylurea	131.6	22810	6
$C_9H_{13}ClN_2O_2$	5-Chloro-3-(1,1-dimethylethyl)-6-methyl-2,4-(1*H*, 3*H*)-pyrimidinedione	174.9	12505	6
$C_9H_{13}ClN_6$	2{[4-Chloro-6-(ethylamino)-1,3,5-triazin-2-yl]-amino}-2-methylpropanenitrile	164.8	41960	6
$C_9H_{16}N_4OS$	*N*-[5-(1, 1-Dimethylethyl)-1,3,4-thiadiazol-2-yl]-*N,N'*-dimethylurea	162.1	29480	6
$C_9H_{16}O_4$	Azelaic acid	106.8	32670	19
C_9H_{18}	*n*-Propylcyclohexane	−94.9	10370	62
$C_9H_{18}N_2O_2S$	3,3-Dimethyl-1-(methylthio)-2-butanone-*O*-methylcarbamoyloxime	57.1	19830	6
$C_9H_{18}N_6$	1,3,5-Tris(dimethylamino)-*s*-triazine	171.2	23010	57
$C_9H_{18}N_6$	1-(Ethylamino)-3,5-bis(dimethylamino)-*s*-triazine	59.8	16740	57
$C_9H_{18}O$	5-Nonanone	−3.9	24930	36
$C_9H_{18}O_2$	Pelargonic acid	12.4	20280	5
C_9H_{20}	*n*-Nonane	−53.5	15470	5
C_9H_{20}	2,2,3,3-Tetramethylpentane	−9.8	2330	63
C_9H_{20}	2,2,4,4-Tetramethylpentane	−66.5	9750	63

TABLE 1 (continued)

Formula	Chemical name	T_{mp}	$\Delta \bar{H}^{fus}$	Ref.
C_9H_{20}	3,3-Diethylpentane	−33.1	10090	63
$C_9H_{20}N_2O$	1,3-Dibutylurea	73.7	14870	10
$C_9H_{20}O_2$	1,9-Nonanediol	46.4	36400	37
$C_{10}H_4Cl_2O_2$	2,3-Dichloro-1,4-naphthalenedione	195.8	28530	6
$C_{10}H_6Cl_4O_4$	Dimethyl-2,3,5,6-tetrachloro-1,4-benzene dicarboxylate	158.5	30225	6
$C_{10}H_7Br$	α-Bromonaphthalene	−1.8	15160	64
$C_{10}H_7Br$	β-Bromonaphthalene	58.8	11970	64
$C_{10}H_7Cl$	α-Chloronaphthalene	−2.5	12900	64
$C_{10}H_7Cl$	β-Chloronaphthalene	58.8	14700	64
$C_{10}H_7I$	α-Iodonaphthalene	6.8	15910	64
$C_{10}H_7I$	β-Iodonaphthalene	54.4	16040	64
$C_{10}H_7NO_2$	α-Nitronaphthalene	56.7	18430	5
$C_{10}H_8$	Naphthalene	78.2	19120	5, 65
$C_{10}H_8ClN_3O$	5-Amino-4-chloro-2-phenyl-3(2*H*)-pyridazinone	206.0	26750	6
$C_{10}H_8O$	α-Naphthol	94.0	23330	5, 6, 66
$C_{10}H_8O$	β-Naphthol	123.0	17510	5, 66
$C_{10}H_9Cl_3O_2$	Methyl 2-(2,4,5-trichlorophenoxy)propionate	87.5	31950	6
$C_{10}H_9Cl_4O_4P$	(*Z*)-2-Chloro-1-(2,4,5-trichlorophenyl)vinyl dimethylphosphate	96.0	35310	6
$C_{10}H_9N$	α-Aminonaphthalene	50.0	14490	5, 66
$C_{10}H_9N$	β-Aminonaphthalene	113.0	23610	66
$C_{10}H_{10}Cl_2O_3$	4-(2,4-Dichlorophenoxy)butyric acid	118.2	38420	6
$C_{10}H_{11}F_3N_2O$	*N*,*N*-Dimethyl-*N*′-[3-(trifluoromethyl)-phenyl]urea	160.9	29820	6
$C_{10}H_{11}ClO_3$	2-(4-Chloro-2-methylphenoxy)propanoic acid	93.0	26430	6
$C_{10}H_{12}ClNO_2$	Isopropyl-3-chlorophenylcarbamate	40.7	17750	6
$C_{10}H_{12}N_3O_3PS_2$	*S*-(3,4-Dihydro-4-oxobenzo[*d*][1,2,3]-triazin-3-ylmethyl)*O*,*O*-dimethyl phosphorodithioate	72.2	27760	6
$C_{10}H_{12}O_3$	Propyl 4-hydroxybenzoate	96.1	6690	54
$C_{10}H_{12}O_3$	4-Ethoxyphenylacetic acid	87.0	23000	41
$C_{10}H_{12}O_3$	4-Methoxyphenylpropionic acid	103.7	28500	41
$C_{10}H_{13}ClN_2$	*N*′-(4-Chloro-2-methylphenyl)-*N*,*N*′-dimethyl methanimidamide	32.1	19370	6
$C_{10}H_{13}NO_2$	Isopropyl phenylcarbamate	86.3	19370	6
$C_{10}H_{13}NO_2$	Propyl 4-aminobenzoate	73.9	20540	52, 54
$C_{10}H_{13}NO_2$	Methyl 4-*N*,*N*-dimethylaminobenzoate	98.6	26070	54
$C_{10}H_{14}$	*n*-Butylbenzene	−87.9	11220	61
$C_{10}H_{14}$	1,2,4,5-Tetramethylbenzene	79.3	21000	5
$C_{10}H_{14}$	1,2,3,4-Tetramethylbenzene	−7.7	11230	5
$C_{10}H_{14}NO_5PS$	*O*,*O*-Diethyl *O*-4-nitrophenyl phosphorothioate	4.9	15720	6
$C_{10}H_{14}O$	Thymol	51.5	17265	5
$C_{10}H_{15}N_5O$	6-Methoxy-*N*,*N*′-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine	90.4	21180	6
$C_{10}H_{16}O$	*d*-Camphor	189.2	15730	6
$C_{10}H_{18}O_4$	Sebacic acid	130.8	40800	19

TABLE 1 (continued)

Formula	Chemical name	T_{mp}	$\Delta \bar{H}^{fus}$	Ref.
$C_{10}H_{20}$	*n*-Butylcyclohexane	−74.7	14160	62
$C_{10}H_{20}N_6$	1-(Methyl-ethylamino)-3,5-bis(dimethylamino)-*s*-triazine	110.8	21300	57
$C_{10}H_{20}N_6O$	1-(Methyl-ethanolamino)-3,5-bis-(dimethylamino)-*s*-triazine	100.1	17320	57
$C_{10}H_{20}O_2$	*n*-Capric acid	32.0	28010	5, 58
$C_{10}H_{22}$	*n*-Decane	−29.7	28780	5
$C_{10}H_{22}O_2$	1,10-Decanediol	72.3	41700	37
$C_{11}H_8O_2$	α-Naphthoic acid	161.0	19890	66
$C_{11}H_8O_2$	β-Naphthoic acid	185.0	23540	66
$C_{11}H_8O_2$	2-Acetyl-1-naphthol	98.6	22520	67
$C_{11}H_8O_2$	1-Acetyl-2-naphthol	63.8	21340	67
$C_{11}H_{10}$	2-Methylnaphthalene	34.4	11970	5
$C_{11}H_{11}ClO_3$	4-(4-Chloro-2-methylphenoxy) butanoic acid	100.3	32020	6
$C_{11}H_{13}NO_4$	2,3-Isopropylidenedioxyphenyl-*N*-methylcarbamate	129.5	29450	6
$C_{11}H_{14}$	1,1-Dimethylindan	−45.8	11990	68
$C_{11}H_{14}$	4,6-Dimethylindan	−16.7	12880	68
$C_{11}H_{14}$	4,7-Dimethylindan	−0.5	13520	68
$C_{11}H_{14}ClNO$	2-Chloro-*N*-isopropyl *N*-phenyl-acetamide	78.2	26050	6
$C_{11}H_{14}O_3$	4-Methoxyphenylbutyric acid	57.7	25300	41
$C_{11}H_{14}O_3$	4-Butoxybenzoic acid	147.7	19100	41
$C_{11}H_{15}NO_2$	Butyl 4-aminobenzoate	57.9	20460	52
$C_{11}H_{15}NO_2S$	4-Methylthio-3,5-xylyl methyl-carbamate	120.6	30360	6
$C_{11}H_{15}NO_3$	2-Isopropoxyphenyl *N*-methyl-carbamate	89.5	22960	6
$C_{11}H_{19}N_5S$	6-(Ethylthio)-*N*, *N*′-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine	104.5	23940	6
$C_{11}H_{20}N_6$	1-(Pyrrolidinyl)-3,5-bis(dimethylamino)-*s*-triazine	129.9	25610	57
$C_{11}H_{20}N_6O$	1-(Morpholinyl)-3,5-bis(dimethylamino)-*s*-triazine	124.2	24690	57
$C_{11}H_{20}N_6S$	1-(Thiomorpholinyl)-3,5-bis(dimethyl-amino)-*s*-triazine	118.0	29080	57
$C_{11}H_{20}O_4$	Undecanedioic acid	111.8	39650	19
$C_{11}H_{21}N_7$	1-(1-Piperizinyl)-3,5-bis(dimethylamino)-*s*-triazine)	108.8	23010	57
$C_{11}H_{22}O_2$	*n*-Undecilic acid	28.3	25100	5
$C_{11}H_{24}$	*n*-Undecane	−25.6	22320	5
$C_{12}Cl_{10}$	Decachlorobiphenyl	304.5	39430	6, 69, 70
$C_{12}HCl_9$	2,2′,3,3′,4,5,5′,6,6′-Nonachloro-biphenyl	182.6	22600	69
$C_{12}H_2Cl_8$	2,2′,3,3′,5,5′,6,6′-Octachlorobi-phenyl	160.6	22800	69
$C_{12}H_3Cl_7$	2,2′,3,3′,4,4′,6-Heptachlorobi-phenyl	122.2	20300	69

TABLE 1 (continued)

Formula	Chemical name	T_{mp}	$\Delta\overline{H}^{fus}$	Ref.
$C_{12}H_4Cl_6$	2,2′,3,3′,4,4′-Hexachlorobiphenyl	151.7	29200	69
$C_{12}H_4Cl_6$	2,2′,3,3′,6,6′-Hexachlorobiphenyl	112.0	21100	69
$C_{12}H_4Cl_6$	2,2′,4,4′,6,6′-Hexachlorobiphenyl	113.5	17500	69
$C_{12}H_5Cl_5$	2,2′,4,5,5′-Pentachlorobiphenyl	76.9	18800	69
$C_{12}H_5Cl_5$	2,3,4,5,6-Pentachlorobiphenyl	124.4	21800	69
$C_{12}H_6Cl_4$	2,2′,4′,5-Tetrachlorobiphenyl	65.9	23400	69
$C_{12}H_6Cl_4$	2,3,4,5-Tetrachlorobiphenyl	90.7	25200	69
$C_{12}H_7Cl_3$	2,4,6-Trichlorobiphenyl	61.1	16500	69
$C_{12}H_7Cl_3$	2,4,5-Trichlorobiphenyl	76.3	22800	69
$C_{12}H_8$	Acenaphthylene	88.9	10960	6
$C_{12}H_8Cl_2$	2,6-Dichlorobiphenyl	34.7	12600	69
$C_{12}H_8O$	Dibenzofuran	82.5	18600	71, 72
$C_{12}H_8O_2$	Xanthone	176.5	26120	51
$C_{12}H_8S$	Dibenzothiophene	97.8	15300	72, 73
$C_{12}H_8S_2$	Thianthrene	155.3	25440	74
$C_{12}H_9Cl$	4-Chlorobiphenyl	75.4	13320	75
$C_{12}H_9Cl$	2-Chlorobiphenyl	32.1	15300	69, 76
$C_{12}H_9N$	Carbazole	243.0	29420	5, 72
$C_{12}H_9NS$	10*H*-Phenothiazine	185.0	26920	6
$C_{12}H_{10}$	Acenaphthene	93.4	21540	65, 77, 91
$C_{12}H_{10}$	Biphenyl	69.0	18600	5, 28, 69, 73, 78
$C_{12}H_{10}N_2$	Azobenzene	67.1	22040	5, 6, 79
$C_{12}H_{10}N_2O$	Azoxybenzene	36.0	17930	5
$C_{12}H_{10}O$	2-Phenylphenol	57.6	13460	6
$C_{12}H_{10}O$	Diphenyl ether	26.6	16160	6
$C_{12}H_{10}O_2$	1-Naphthaleneacetic acid	132.1	22260	6
$C_{12}H_{11}N$	Diphenylamine	53.0	17860	5, 6, 27
$C_{12}H_{11}NO$	1-Naphthaleneacetamide	183.2	32820	6
$C_{12}H_{11}NO_2$	1-Naphthyl methylcarbamate	143.1	24510	6
$C_{12}H_{12}$	1,4-Dimethylnaphthalene	6.8	15900	80
$C_{12}H_{12}$	2,3-Dimethylnaphthalene	104.8	25100	80
$C_{12}H_{12}$	2,6-Dimethylnaphthalene	110.2	25060	77
$C_{12}H_{12}$	2,7-Dimethylnaphthalene	95.7	23350	77
$C_{12}H_{12}$	1,8-Dimethylnaphthalene	63.2	15770	77
$C_{12}H_{12}N_2$	Hydrazobenzene	134.0	17650	5
$C_{12}H_{13}NO_2S$	5,6-Dihydro-2-methyl-*N*-phenyl-1,4-oxathiin-3-carboxamide	91.0	28770	6
$C_{12}H_{16}$	Cyclohexylbenzene	7.3	15300	73
$C_{12}H_{16}Cl_2N_2O$	*N*-Butyl-*N*′-(3,4-dichlorophenyl)-*N*-methylurea	101.1	27230	6
$C_{12}H_{17}NO_2$	Pentyl 4-aminobenzoate	51.9	23930	52
$C_{12}H_{18}O_2$	4-Hexylresorcinol	68.3	19040	81
$C_{12}H_{19}N_4O_2$	3-Cyclohexyl-6-(dimethylamino)-1-methyl-1,3,5-triazine-2,4-(1*H*,3*H*)-dione	116.4	20360	6
$C_{12}H_{22}N_6$	1-(Piperidinyl)-3,5-bis(dimethylamino)-*s*-triazine	88.3	23220	57
$C_{12}H_{22}O_4$	Dodecanedioic acid	129.3	50570	19, 58
$C_{12}H_{23}N_7$	1-(4′-Formyl-1-piperizinyl)-3,5-bis(dimethylamino)-*s*-triazine	88.0	20420	57

TABLE 1 (continued)

Formula	Chemical name	T_{mp}	$\Delta\bar{H}^{fus}$	Ref.
$C_{12}H_{24}O_2$	*n*-Lauric acid	43.2	36640	5
$C_{12}H_{26}$	*n*-Dodecane	−9.6	36580	5
$C_{13}H_6Cl_6O_2$	2,2′-Methylenebis(3,4,6-trichlorophenol)	164.4	33260	6
$C_{13}H_8Cl_2O$	*p*,*p*′-Dichlorobenzophenone	146.8	30120	27
$C_{13}H_8O$	9-Fluorenone	83.2	18120	82
$C_{13}H_9N$	Acridine	179.2	19700	72
$C_{13}H_{10}$	Fluorene	114.8	19580	65, 77
$C_{13}H_{10}O$	Benzophenone	47.9	18190	5, 83
$C_{13}H_{10}O$	Xanthene	100.5	19200	72
$C_{13}H_{12}N_2O$	1,3-Diphenylurea	238.8	34600	48
$C_{13}H_{13}N$	Benzylaniline	32.4	16760	5
$C_{13}H_{16}F_3N_3O_4$	2,6-Dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)benzenamine	48.2	22320	6
$C_{13}H_{16}F_3N_3O_4$	*N*-Butyl-*N*-ethyl-2,6-dinitro-4-trifluoromethylaniline	65.3	36500	6
$C_{13}H_{18}$	1,1,4,6-Tetramethylindan	0.4	15740	68
$C_{13}H_{18}$	1,1,4,7-Tetramethylindan	−27.6	11280	68
$C_{13}H_{24}N_6$	1-(Hexamethyleneimine)-3,5-bis(dimethylamino)-*s*-triazine	62.6	16320	57
$C_{13}H_{24}O_4$	Tridecanedioic acid	114.3	45300	19
$C_{13}H_{28}O$	Tri-*tert*-butylmethanol	117.0	3430	84
$C_{14}H_7ClF_3NO_5$	5-[2-Chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoic acid	163.5	37670	6
$C_{14}H_8Cl_4$	1,1-Dichloro-2,2-bis(4-chlorophenyl)-ethylene	87.3	23550	6
$C_{14}H_8O_2$	Anthraquinone	284.8	32650	5, 6
$C_{14}H_9Cl_5$	1,1′-(2,2,2-Trichloroethylidene)bis(4-chlorobenzene)	108.9	26280	6
$C_{14}H_9Cl_5O$	2-Chloro-α-(4-chlorophenyl)-α-(trichloromethyl)benzene-methanol	123.1	25200	6
$C_{14}H_{10}$	Anthracene	219.5	28830	5, 65
$C_{14}H_{10}$	Phenanthrene	99.2	16470	5, 6, 65, 77
$C_{14}H_{10}Cl_4$	1,1′-(2,2-Dichloroethylidene)bis(4-chlorobenzene)	109.0	27310	6
$C_{14}H_{10}O_2$	Benzil	95.2	19760	5
$C_{14}H_{12}$	*trans*-Stilbene	125.0	27400	5, 79
$C_{14}H_{14}O_3$	2-Pivaloylindan-1,3-dione	108.4	25990	6
$C_{14}H_{28}O_2$	Myristic acid	54.0	45380	5, 58
$C_{15}H_{11}ClF_3NO_4$	2-Chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene	85.6	30070	6
$C_{15}H_{15}ClN_2O_2$	3-[4-(4-Chlorophenoxy)phenyl]-1,1-dimethylurea	152.6	34870	6
$C_{15}H_{15}N$	*N*-Isopropylcarbazole	122.0	17730	85
$C_{16}H_{10}$	Pyrene	151.2	17110	65, 86
$C_{16}H_{10}$	Fluoranthene	107.8	18870	65
$C_{16}H_{14}Cl_2O_4$	Methyl 2-(4-(2,4-Dichlorophenoxy)-phenoxy)propionate	41.3	27080	6
$C_{16}H_{15}Cl_3O_2$	1,1′-(2,2,2-Trichloroethylidene)bis[4-methoxybenzene]	87.5	23880	6

TABLE 1 (continued)

Formula	Chemical name	T_{mp}	$\Delta \overline{H}^{fus}$	Ref.
$C_{16}H_{17}NO$	*N*,*N*-Dimethyl-2,2-diphenylacetamide	133.9	25430	6
$C_{16}H_{24}N_6$	1-(Methylphenethylamino)-3,5-bis(dimethylamino)-*s*-triazine	61.0	20040	57
$C_{16}H_{32}$	*n*-Decylcyclohexane	−1.7	38590	62
$C_{16}H_{32}O_2$	Palmitic acid	61.8	42040	5
$C_{16}H_{34}O$	1-Hexadecanol	49.3	34290	5
$C_{17}H_{16}Br_2O_3$	Isopropyl 4,4′-dibromobenzilate	74.9	24550	6
$C_{18}H_{12}$	Chrysene	258.2	26150	65
$C_{18}H_{12}$	Triphenylene	200.3	25100	65
$C_{18}H_{12}$	1,2-Benzanthracene	161.1	21380	65
$C_{18}H_{12}$	3,4-Benzophenanthrene	61.5	16310	65
$C_{18}H_{14}$	*p*-Terphenyl	210.1	35500	78
$C_{18}H_{14}O_3$	Cinnamic anhydride	48.0	32770	5
$C_{18}H_{15}OP$	Triphenylphosphine *P*-oxide	158.7	24220	87
$C_{18}H_{15}O_4P$	Triphenyl phosphate	49.3	29610	88
$C_{18}H_{15}P$	Triphenylphosphine	81.2	19690	87
$C_{18}H_{20}Cl_2$	1,1′-(2,2-Dichloroethylidene)bis(4-ethylbenzene)	58.5	23340	6
$C_{18}H_{34}O_2$	Elaidic acid	44.4	61550	5
$C_{18}H_{36}O_2$	Stearic acid	68.8	56590	5, 58
$C_{18}H_{38}$	*n*-Octadecane	28.2	61390	5
$C_{19}H_{40}$	*n*-Nonadecane	32.1	45820	5
$C_{20}H_{12}$	Perylene	280.7	31750	65
$C_{20}H_{12}$	1,2-Benzopyrene	181.2	16560	65
$C_{20}H_{12}$	3,4-Benzopyrene	181.0	17320	65
$C_{20}H_{18}O_2Sn$	(Acetyloxy)triphenylstannane	124.5	41920	6
$C_{20}H_{40}O_2$	*n*-Eicosanoic acid	75.1	69200	58
$C_{20}H_{42}$	*n*-Eicosane	36.8	69880	5
$C_{21}H_{16}$	1,2′-Dinaphthylmethane	96.4	30550	77
$C_{21}H_{44}$	*n*-Heneicosane	40.5	47700	5
$C_{22}H_{12}$	1,12-Benzoperylene	281.0	17370	65, 80
$C_{22}H_{12}$	*o*-Phenylenepyrene	162.0	21505	80
$C_{22}H_{14}$	1,2:3,4-Dibenzanthracene	280.3	25820	65
$C_{22}H_{14}$	1,2:5,6-Dibenzanthracene	271.0	31160	65
$C_{22}H_{46}$	*n*-Docosane	44.4	49960	5
$C_{23}H_{48}$	*n*-Tricosane	47.6	41760	5
$C_{24}H_{12}$	Coronene	437.3	19200	80
$C_{24}H_{14}$	3,4:9,10-Dibenzopyrene	283.6	27870	65
$C_{24}H_{14}$	1,2:3,4-Dibenzopyrene	228.0	24680	65
$C_{24}H_{14}$	1,2:4,5-Dibenzopyrene	247.0	30500	65
$C_{24}H_{18}$	*p*-Quarterphenyl	314.0	37800	78
$C_{24}H_{50}$	*n*-Tetracosane	50.9	54890	5
$C_{25}H_{52}$	*n*-Pentacosane	53.7	57740	5
$C_{26}H_{14}$	1,12-Phenyleneperylene	268.3	17280	80
$C_{27}H_{56}$	*n*-Heptacosane	59.0	60430	5
$C_{28}H_{58}$	*n*-Octacosane	61.4	64650	5

interactions, which depend on the types of functional group present in the molecule, and in the case of crystalline organic compounds, are reflected in the magnitude of the enthalpy of fusion and melting temperature.

From a thermodynamic standpoint, prediction of the aqueous mole fraction solubilities, X_A^{sat}, of a crystalline non-electrolyte requires a prior knowledge of the solute's melting point temperature T_{mp} and molar enthalpy of fusion $\Delta\overline{H}_A^{fus}$. In the absence of heat capacity data, the last two terms in the equation

$$\ln\left(\gamma_A^{sat} X_A^{sat}\right) = -\frac{\Delta\overline{H}_A^{fus}\left(T_{mp} - T\right)}{RTT_{mp}} + \frac{\Delta\overline{C}_p\left(T_{mp} - T\right)}{RT} - \left(\Delta\overline{C}_p/R\right)\ln\left(T_{mp}/T\right) \tag{1}$$

can often be set equal to zero, i.e. $\Delta\overline{C}_p = 0$, with only slight loss in predictive accuracy. Group contribution methods, such as the UNIFAC and ASOG models, enable activity coefficients, γ_A^{sat}, to be estimated from only structural information and tabulated group parameters. Both group contribution methods are discussed in detail in monographs by Acree [1] and Prausnitz et al. [2]. Thermodynamic modeling has not yet advanced to the point where fusion enthalpies can be estimated accurately, although there have been two fairly recent attempts in this area involving select classes of organic compounds [3,4].

To provide a convenient reference source for enthalpy of fusion data, published values taken from the chemical literature are reported in Tables 1 and 2. Compounds are arranged according to molecular formula, beginning with increasing carbon and hydrogen atom numbers. Other substituent atoms follow alphabetically. Tabulated values are based either on a single measurement or, in some instances, on the average of several independently determined values. Care was taken to eliminate typographical errors, but readers should be aware that in a compilation of this magnitude a few errors will undoubtedly occur. Literature references are given in the last column to indicate actual sources consulted. It is hoped that the tabulation will not only provide input $\Delta\overline{H}^{fus}$ values for aqueous solubility predictions, but will form a data base for developing better estimational schemes for fusion enthalpies.

TABLE 2

Molar enthalpies of fusion (J mol^{-1}) and melting point temperature (°C)

Formula	Chemical name	T_{mp}	$\Delta \bar{H}^{fus}$	Ref.
$C_2H_7AsO_2$	Hydroxydimethylarsine	197.7	24455	6
$C_3H_4O_2$	β-Propiolactone	−33.3	9410	18
$C_5H_2Cl_3O$	3,5,6-Trichloro-2-pyridinol	174.9	25790	6
$C_7H_4Cl_4O_4$	Methyltetrachloroterephthalic acid ester	171.1	16890	6
$C_7H_{13}N_3O_3S$	*N*,*N*-Dimethyl-2-methylcarbamoyloxyimino-2-(methylthio) acetamide	99.1	30170	6
$C_9H_6Cl_2N_2O_3$	2-(3,4-Dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione	123.2	29500	6
$C_9H_9Cl_2NO$	3′,4′-Dichloropropionanilide	90.5	18260	6
$C_9H_9NO_4$	[(Benzoylamino)oxy]acetic acid	143.8	31460	6
$C_9H_{10}Cl_2N_2O_2$	*N*′-(3,4-Dichlorophenyl)-*N*-methoxy-*N*-methylurea	92.6	26560	6
$C_9H_{11}ClN_2O_2$	*N*′-(4-Chlorophenyl)-*N*-methoxy-*N*-methylurea	80.2	22540	6
$C_9H_{12}N_4O_2$	8-Ethyltheophylline	272.1	37200	89
$C_9H_{16}ClN_5$	2-Chloro-4,6-bis(isopropylamino)-1,3,5-triazine	217.1	41865	6
$C_{10}H_9Cl_2NO$	*N*-(3,4-Dichlorophenyl)-2-methyl-2-propenamide	122.3	32040	6
$C_{10}H_9Cl_3O_3$	4-(2,4,5-Trichlorophenoxy)butanoic acid	113.5	30275	6
$C_{10}H_{11}F_3N_2O_3S$	*N*-(4-Methyl-3{[trifluoromethyl)sulfonyl]amino}phenyl) acetamide	182.5	40470	6
$C_{10}H_{12}N_2O_3S$	3-(1-Methylethyl)-(1*H*)-2,1,3-benzothiadiazin-4(3*H*)-one 2,2-dioxide	139.3	21765	6
$C_{10}H_{13}NO_2$	3,4-Dimethylphenyl methylcarbamate	77.7	24965	6
$C_{10}H_{14}N_4O_2$	8-Propyltheophylline	261.1	33300	89
$C_{10}H_{16}Cl_3NOS$	*S*-2,3,3-Trichloroallyl diisopropylthiocarbamate	33.2	27110	6
$C_{11}H_{16}N_4O_2$	8-*n*-Butyltheophylline	236.0	32300	89
$C_{11}H_{16}N_4O_2$	8-*tert*-Butyltheophylline	129.1	48200	89
$C_{11}H_{19}N_3O$	5-Butyl-2-ethylamino-6-methylpyrimidin-4-ol	159.3	20320	6

$C_{12}H_6Cl_4O_2S$	1,2,4-Trichloro-5-[(4-chlorophenyl)sulfonyl]benzene	146.7	28940	6
$C_{12}H_8Cl_2O_3S$	4-Chlorophenyl 4-chlorobenzene sulfonate	86.9	23630	6
$C_{12}H_9ClO_3S$	4-Chlorophenylbenzene sulfonate	59.1	21440	6
$C_{12}H_{10}S$	Thioxanthene	128.6	26100	72
$C_{12}H_{15}NO_3$	2,3-Dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate	153.1	30330	6
$C_{12}H_{16}NO_2$	5-Isopropyl-*m*-tolylmethylcarbamate	88.1	23040	6
$C_{12}H_{18}N_2O$	*N*,*N*-Dimethyl-*N'*-[4-(1-methylethyl)phenyl]urea	157.3	33870	6
$C_{12}H_{18}N_2O_2$	3,5-Dimethyl-4-(dimethylamino)phenyl methylcarbamate	88.5	18370	6
$C_{12}H_{18}N_4O_2$	8-Pentyltheophylline	225.2	35100	89
$C_{13}H_7F_3N_2O_5$	2-Nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)benzene	91.4	18440	6
$C_{13}H_{19}N_3O_4$	*N*-(1-Ethylpropyl)-2,6-dinitro-3,4-xylidine	54.3	25190	6
$C_{13}H_{20}N_4O_2$	8-Hexyltheophylline	202.5	26100	89
$C_{14}H_9Cl_2NO_5$	Methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate	85.2	26310	6
$C_{14}H_{10}Cl_2O_2$	bis(4-Chlorophenyl)acetic acid	167.1	31660	6
$C_{14}H_{20}$	Cyclotetradecadiyne	96.9	22550	3
$C_{14}H_{20}ClNO_2$	2-Chloro-*N*-(2,6-diethylphenyl)-*N*-(methoxymethyl)acetamide	42.7	25310	6
$C_{14}H_{22}N_4O_2$	8-Heptyltheophylline	199.5	33000	89
$C_{14}H_{28}$	Cyclotetradecane	54.9	28700	3
$C_{16}H_{14}Cl_2O_3$	Ethyl 4-chloro-α-(4-chlorophenyl)-α-hydroxybenzene acetate	37.2	23480	6
$C_{16}H_{16}N_2O_4$	Ethyl-3-phenylcarbamoyloxyphenylcarbamate	121.0	32750	6
$C_{16}H_{16}N_2O_4$	Methyl-3-*m*-tolylcarbamoyloxyphenylcarbamate	150.6	39620	6
$C_{17}H_{12}O_2$	4-Benzoyl-1-naphthol	167.4	28640	90
$C_{17}H_{12}O_2$	1-Benzoyl-2-naphthol	140.9	31350	90
$C_{17}H_{12}O_2$	2-Benzoyl-1-naphthol	70.7	20180	90
$C_{18}H_{18}O_3$	Butyl 9-hydroxy-9*H*-fluorene-9-carboxylate	70.7	25555	6
$C_{18}H_{30}N_4O_2$	8-Unadecyltheophylline	160.3	25800	89
$C_{22}H_{38}N_4O_2$	8-Pentadecyltheophylline	140.5	27200	89

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