Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)	
	497.7	28.67	0	57.6	74.0	28.67	36.8 [221]	C_{13}
		6*A10+6*A12+3*A21+A31+A60						
$C_{13}H_8Cl_2O$		*p, p′*-dichlorobenzophenone						
	420	30.12	0	71.71	66.3	30.12	27.9 [215]	C_{13}
		2*A22*C22+A35+8*A10+4*A12						
$C_{13}H_8O$		xanthene						
	373.7	19.2	0	51.38	56.0	19.2	20.9 [215]	C_{13}
		A14+3*A15+2*A19+8*A10+A112+2*A19						
$C_{13}H_8O$		9-fluorenone						
	356.4	18.12	0	50.84	49.7	18.12	17.7 [215]	C_{13}
		8*A10+A14+2*A15+2*A19+A114+2*A19						
$C_{13}H_8OS$		thioxanthone						
	487.9	35.5	0	72.76	56.3	35.5	27.5 [160]	C_{13}
		A14+3*A15+4*A19+A114+A131+8*A10						
$C_{13}H_8O_2$		xanthone						
	449.7	26.12	0	58.08	54.6	26.12	24.6 [216]	C_{17}
		A14+3*A15+4*A19+A112+A114+8*A10						
$C_{13}H_9Cl_3N_2O$		benzoic acid, 2,4,6-trichlorophenyl hydrazide						
	439.7	32.71	0	74.4	59.2	32.71	26.0 [221]	C_{13}
		7*A10+5*A12+3*A22*D22+A60+A44						
$C_{13}H_9F_3N_2O_2$		2-[[3-(trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid						
	476	38	0	79.83	72.8	38	34.6 [85]	C_{13}
		3*A25+A4*B4+7*A10+3*A12+A11+A44+A41+A36						
$C_{13}H_9N$		acridine						
	383.2	18.58	0	48.48	47.7	18.58	18.3 [284]	C_{13}
		9*A10+2*A12+A41+2*A12						
$C_{13}H_9N$		7,8-benzoquinoline						
	324.1	14.1	0	43.51	47.7	14.1	15.5 [216]	C_{13}
		9*A10+4*A12+A41						
$C_{13}H_9N$		phenanthridine						
	354	0.02	0.06					
	379.7	22.83	60.12	60.18	47.7	22.85	18.1 [216]	C_{13}
		9*A10+4*A12+A41						
$C_{13}H_9N_2$		2-phenylbenzimidazole						
	572.2	22.18	0	38.75	65.9	22.18	37.7	C_{13}
		9*A10+A118+A121+A14+2*A15+3*A19+A12						
$C_{13}H_{10}$		fluorene						
	387.9	19.58	0	50.48	51.0	19.58	19.8 [216]	C_{13}
		8*A10+A14+2*A15+4*A19						
$C_{13}H_{10}BrCl_2O_2PS$		O-(4-bromo-2,5-dichlorophenyl)O-methyl phenylphosphonothioate						
	345.6	31.35	0	90.73	87.2	31.35	30.1 [221]	C_{13}
		7*A10+5*A12+A1+2*A22*D22+A21+A81						
$C_{13}H_{10}Cl_2S$		*p*-chlorobenzyl *p*-chlorophenyl sulfide						
	343.8	32.22	0	93.71	68.9	32.22	23.7 [232]	C_{13}
		8*A10+3*A12+A11+2*A22*D22+A2+A84						
$C_{13}H_{10}N_2$		diphenylcarbodiimide						
	287.4	18.55	0	64.54	52.9	18.55	15.2 [227]	C_{13}
		10*A10+2*A12+2*A42+A9						
$C_{13}H_{10}N_2O$		1,3-diphenylurea						
	512	34.6	0	67.58	60.7	34.6	31.1 [215]	C_{13}
		10*A10+2*A12+A66						
$C_{13}H_{10}O$		benzophenone						
	321.0	18.19	0	56.67	63.8	18.19	20.5 [80]	C_{13}
		10*A10+2*A12+A35						
$C_{13}H_{10}S$		thioxanthene						
	401.8	26.1	0	64.96	57.6	26.1	23.2 [215]	C_{13}
		A14+3*A15+2*A19+2*A19+A131+8*A10						
$C_{13}H_{11}N$		N-methylcarbazole						
	362.5	17.15	0	47.32	49.3	17.15	17.9 [216]	C_{13}
		A14+2*A15+2*A19+2*A19+A119+A1+8*A10						
$C_{13}H_{11}NO$		benzanilide						
	436.5	29.61	0	67.84	60.6	29.61	26.5 [216]	C_{13}
		10*A10+2*A12+A60						
$C_{13}H_{12}$		diphenylmethane						
	298.3	18.58	0	62.34	62.1	18.58	18.5 [216]	C_{13}
		10*A10+A2+2*A11						

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{13}H_{12}NO$		1,3-diphenylurea					
	512.1	34.62	0	67.6	60.7	34.62	31.1 [216]
		10*A10+2*A12+A66					
$C_{13}H_{12}O$		diphenylcarbinol					
	338.5	23	0	67.93	46.9	23	15.9 [216]
		10*A10+2*A11+A3*B3+A30					
$C_{13}H_{13}BrS$		2-*n*-propyl-5-(4-bromophenyl)thiophene					
	360.4	15.7	0	43.56	58.7	15.7	21.2 [251]
		A14+2*A15+A131+2*A19+2*A19+A1+2+4*A10+2*A12+A21					
$C_{13}H_{13}N$		N-benzylaniline					
	305.6	16.76	0	54.84	85.6	16.76	26.2 [215]
		10*A10+A12+A11+A45+A2					
$C_{13}H_{13}NO_2$		(*dl*) 2-(1-naphthoxy)propionamide					
	445	37.66	0	84.62	69.8	37.66	31.1 [273]
		7*A10+3*A12+A32+A3*B3+A1+A61					
$C_{17}H_{13}NO_2$		(*d*) 2-(1-naphthoxy)propionamide					
	475	38.07	0	80.16	69.8	38.07	33.2 [273]
		7*A10+2*A12+A32+A3*B3+A1+A61+A12					
$C_{13}H_{14}N_2$		*bis*-(4-aminophenyl)methane					
	363.7	9.23	0	25.36	75.0	9.23	27.3 [216]
		8*A10+2*A11+2*A12+2*A45+A2					
$C_{13}H_{15}N$		1,2,3,4-tetrahydro-9-methylcarbazole					
	162	0.08	0.5				
	323.8	14.67	45.29	45.8	39.2	14.75	12.7 [15]
		2*A14+3*A15+2*A19+2*A19+4*A10+A119					
$C_{13}H_{15}NO_2$		3,4-dihydro-6-methyl-2H-pyran-5-carboxanilide					
	381.1	19.21	0	50.4	69.8	19.21	26.6 [221]
		A14+3*A15+A112+2*A19+A60+5*A10+A12+A1					
$C_{13}H_{15}N_3O_2$		3-methyl-1-phenyl-1H-pyrazol-5yl dimethylcarbamate					
	324.3	21.39	0	65.96	65.9	21.39	21.4 [221]
		A14+2*A15+3*A1+5*A10+A12+A68+3*A19+A12+A118					
$C_{13}H_{16}F_3N_3O_4$		2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)benzenamine					
	321.4	22.32	0	69.45	76.6	22.32	24.6 [215]
		2*A10+A11+3*A12+2*A50+A43+3*A25 +A4*B4+2*A1+4*A2					
$C_{13}H_{16}F_3N_3O_4$		N-butyl-N-ethyl-2,6-dinitro-4-trifluoromethylaniline					
	338.5	36.5	0	107.83	76.6	36.5	25.9 [215]
		2*A10+A11+3*A12+2*A50+A43+3*A25+A4*B4+2*A1+4*A2					
$C_{13}H_{18}$		1,1,4,6-tetramethylindane					
	273.6	15.74	0	57.53	47.6	15.74	13.0 [215]
		4*A1+2*A10+2*A11+A14+2*A15+A17+2*A19					
$C_{13}H_{18}$		1,1,4,7-tetramethylindane					
	245.6	11.28	0	45.93	47.6	11.28	11.7 [215]
		4*A1+2*A10+2*A11+A14+2*A15+A17+2*A19					
$C_{13}H_{18}ClNO$		N-(4-chlorophenyl)-2,2-dimethylpentanamide					
	360.2	23.31	0	64.71	76.5	23.31	27.6 [221]
		3*A1+2*A2+A4*B4+4*A10+2*A12+A22*B22+A60					
$C_{13}H_{18}ClNO$		N-(3-chloro-4-methylphenyl)-2-methylpentanamide					
	353.2	16.35	0	46.28	72.6	16.35	25.6 [221]
		3*A1+2*A2+2*A12+A11+A3*B3+3*A10+A60+A22*B22					
$C_{13}H_{18}N_2O_2$		3-cyclohexyl-6,7-dihydro-1H-cyclopentapyrimidine-2,4-(3H,5H)-dione					
	584.3	42.31	0	72.41	64.0	42.31	37.4 [221]
		3*A14+6*A15+A16+A124+A125+2*A19					
$C_{13}H_{18}O_5S$		*dl*-2-ethoxy-2,3-dihydro-3,3-dimethyl-5-benzofuranyl methanesulfonate					
	344.1	26.25	0	76.28	68.3	26.25	23.5 [221]
		A14+2*A15+A19+A19+A17+A16+A122+4*A1+A2+3*A10+A12+A89					
$C_{13}H_{19}NO_2$		hexyl N-phenylcarbamate					
	328	32.76	0	100	93.4	32.76	30.7 [102]
		5*A10+A12+A1+5*A2+A69					
$C_{13}H_{19}N_3O_4$		N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine					
	327.5	25.19	0	76.92	70.7	25.19	23.1 [215]
		4*A1+2*A2+A3*B3+A44+2*A50+3*A12+2*A11+A10					
$C_{13}H_{21}N_2O$		N,N-dimethyl-N′-(octahydro-4,7-methano-1H-inden-5-yl)urea					
	436.5	21.74	0	49.81	65.5	21.74	28.6 [221]
		3*A14+A15+5*A16+2*A1+A64					
$C_{13}H_{22}$		1,3,5-trimethyladamantane					
	228.2	6.3	27.61				

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
	253.6	1.73	6.82	34.43	38.2	8.03	9.7
		3*A14+A15+A16+3*A17+3*A1					[146]
$C_{13}H_{22}O_3$		3,3,7,7-tetramethylnonanedioic anhydride					
	396.2	20.5	0	51.75	62.8	20.5	24.9
		A14+7*A15+4*A1+2*A17+A117					[109]
$C_{13}H_{24}N_6$		1-(hexamethyleneimine)-3,5-bis(dimethylamino)-*s*-triazine					
	335.8	16.32	0	48.6	65.0	16.32	21.8
		A14*4*A15+A119+4*A1+2*A43+3*A12+3*A41					[242]
$C_{13}H_{24}O_2$		tridecanolactone					
	290.6	18.16	62.37				
	300.4	9.08	30.21	92.55	77.2	27.24	23.2
		A14+11*A15+A115					[216]
$C_{13}H_{24}O_4$		tridecanedioic acid					
	387.5	45.3	0	116.9	134.9	45.3	52.3
		11*A2*B2+2*A36*B36					[216]
$C_{13}H_{26}$		cyclotridecane					
	285.6	0.9	3.15				
	297.6	7.4	24.87	28.02	70.4	8.3	20.9
		A14+10*A15					[181]
$C_{13}H_{26}$		*n*-heptylcyclohexane					
	232.8	22.22	0	95.43	90.1	22.22	21.0
		A14+A16+A1+6*A2+3*A15					[216]
$C_{13}H_{26}O_2$		tridecanoic acid					
	307.1	8.72	28.41				
	315.0	33.74	107.11	135.52	133.6	42.47	42.1
		11*A2*B2+A1+A36					[216]
$C_{13}H_{26}O_2Si_3$		1,1,1,3,5,5,5-heptamethyl-3-phenyltrisiloxane					
	226.8	18.29	0	80.64	80.8	18.29	18.3
		7*A1+5*A10+A12+2*A32+3*A109					[216]
$C_{13}H_{27}NO_2$		3(*n*-nonylamino)-1,2-propanediol					
	343.2	53.2	0	155.01	125.5	53.2	43.1
		A1+8*A2*B2+A44+2*A30*C30+A3*B3+2*A2					[217]
$C_{13}H_{28}$		*n*-tridecane					
	255	7.66	30.04				
	267.8	28.49	106.27	136.31	137.8	36.15	36.9
		2*A1+11*A2*B2					[216]
$C_{13}H_{28}O$		tri-*tert*-butylmethanol					
	302	7.2	23.84				
	390	3.43	8.379	32.64	32.6	10.63	12.7
		9*A1+3*A4+A30+A4*B4					[216]
$C_{13}H_{28}O$		tridecanol					
	304.6	45.1					
	304.5	41.42	138.9				
	303.5	23.3	76.99				
	301.6	3.6	12.13				
	305.8	22.09	72.38				
	306.6	18.74	61.09	148.11	131.3	45.02	40.3
		A1+12*A2*B2+A30					[224]
$C_{13}H_{28}O_2S$		3(*n*-decylthio)-1,2-propanediol					
	291.9	17.3	59.27				
	311.9	17.3	55.47	114.73	142.3	34.6	44.4
		A1+9*A2*B2+A84+2*A30*C30+A3*B3+2*A2					[217]
$C_{13}H_{28}O_2$		3(*n*-decyloxy)-1,2-propanediol					
	311	38.9	0	125.08	144.9	38.9	45.1
		A1+9*A2*B2+A32+2*A30*C30+A3*B3+2*A2					[217]
$C_{13}H_{29}NO_2$		3(*n*-decylamino)-1,2-propanediol					
	346.6	54.8	0	158.11	134.9	54.8	46.8
		A1+9*A2*B2+A44+2*A30*C30+2*A2+A3*B3					[217]
$C_{14}H_7ClF_3NO_5$		5-[2-chloro-4-(trifluoromethyl)phenoxyl]-2-nitrobenzoic acid					
	436.6	37.67	0	86.27	83.0	37.67	36.2
		6*A10+A11+5*A12+A22*G22+A36*F36+A32+A50+A4*B4+3*A25					[221]
$C_{14}H_7ClO_2$		2-chloroanthraquinone					
	483.0	39	0	80.74	53.3	39	25.7
		A14+3*A15+4*A19+2*A114+A22*C22+A12+7*A10					[216]
$C_{14}H_8Cl_4$		1-chloro-2-(2,2-dichloro-1-(4-chlorophenylethenyl)benzene					
	349.8	23.84	0	68.17	72.7	23.84	25.4
		8*A10+4*A12+A7+A7+4*A22*D22					[221]
$C_{14}H_8Cl_4$		1,1-dichloro-2,2-bis(4-chlorophenyl)ethylene					
	360.4	23.55	0	65.33	72.7	23.55	26.2
		8*A10+4*A12+A7+A7+4*A22*D22					[221]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
$C_{14}H_8O_2$		anthraquinone					
	555	32.57	0	58.7	52.0	32.57	29.0
		3*A15+A14+8*A10+4*A19+2*A114					[216]
$C_{14}H_9ClF_2N_2O_2$		N-[[(4-chlorophenylamino]carbonyl]-2,6-difluorobenzamide					
	499.5	55.99	0	112.08	66.8	55.99	33.4
		7*A10+5*A12+2*A24+A22*E22+2*A60					[221]
$C_{14}H_9Cl_2NO_3$		methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate					
	358.3	26.31	0	73.44	79.7	26.31	28.5
		6*A10+6*A12+2*A22*E22+A50+A32+A38+A1					[215]
$C_{14}H_9Cl_3$		1-chloro-2,2-(bis-(4-chlorophenyl)ethylene					
	337.9	25.52	0	75.53	71.2	25.52	24.0
		8*A10+4*A12+A6*B6+A7+3*A22*C22					[232]
$C_{14}H_9Cl_5$		1,1-(2,2,2-trichloroethylidene)bis(4-chlorobenzene)					
	382.1	26.28	0	68.78	66.9	26.28	25.5
		5*A22*E22+A4*B4+2*A12+2*A11+8*A10+A3					[215]
$C_{14}H_9Cl_5$		1-chloro-2-(2,2,2-trichloro-1-(4-chlorophenyl)ethyl)benzene					
	345.8	23.09	0	66.78	66.9	23.09	23.1
		8*A10+2*A12+2*A11+5*A22*E22+A3+A4*B4					[221]
$C_{14}H_9Cl_5O$		2-chloro-α-(4-chlorophenyl)-α-(trichloromethyl)benzenemethanol					
	396.3	25.2	0	63.61	83.1	25.2	32.9
		8*A10+2*A11+2*A12+2*A4*B4+5*A22*F22+A30*F30					[215]
$C_{14}H_9Cl_5O$		4-chloro-α-(4-chlorophenyl)-α-(trichloromethyl)benzenemethanol					
	347.2	19.56	0	56.35	83.1	19.56	28.9
		8*A10+2*A11+2*A12+2*A4*B4+5*A22*F22+A30*F30					[221]
$C_{14}H_9NO_4PS$		O-ethyl O-(4-nitrophenyl)phenylphosphonothioate					
	308.2	25.05	0	81.29	91.9	25.05	28.3
		9*A10+3*A12+A50+A1+A2+A81					[221]
$C_{14}H_9NO_2$		1-aminoanthraquinone					
	524.2	28.78	0	54.9	58.5	28.78	30.7
		A14+3*A15+2*A114+4*A19+7*A10+A45+A12					[13]
$C_{14}H_{10}$		phenanthrene					
	347.5	0.22	0.63				
	372.4	16.46	44.21	44.83	44.2	16.68	16.5
		10*A10+4*A12					[216]
$C_{14}H_{10}$		anthracene					
	488.9	29.37	0	60.08	44.2	29.37	21.6
		10*A10+4*A12					[216]
$C_{14}H_{10}$		diphenylacetylene					
	334	20.5	0	61.4	53.7	20.5	17.9
		10*A10+2*A9+2*A12					
$C_{14}H_{10}Cl_2O_2$		bis(4-chlorophenyl)acetic acid					
	440.2	31.66	0	71.92	77.7	31.66	34.2
		8*A10+2*A12+2*A11+A3*B3+2*A22*C22+A36*C36					[215]
$C_{14}H_{10}Cl_4$		1,1′-(2,2-dichloroethylidenebis(4-chlorobenzene)					
	382.1	27.31	0	71.48	63.9	27.31	24.4
		8*A10+2*A11+2*A12+A3*B3+4*A22*D22					[215]
$C_{14}H_{10}N_2O_2$		1,4-diaminoanthraquinone					
	484.2	24.2	0	49.98	65.0	24.2	31.5
		A14*3*A15+2*A114+4*A19+6*A10+2*A45+2*A12					[13]
$C_{14}H_{10}O$		anthrone (some decomposition upon melting)					
	429	26.8	0	62.47	53.4	26.8	22.9
		A14+3*A15+2*A19+2*A19+8*A10+A114					[82]
$C_{14}H_{10}O_2$		benzil					
	84	0.04	0.5				
	368	23.56	64.02	64.52	68.4	23.6	25.2
		10*A10+2*A12+2*A35					[216]
$C_{14}H_{10}O_3$		benzoic anhydride					
	313.2	17.15	0	54.77	69.2	17.15	21.7
		10*A10+2*A12+A39					[287]
$C_{14}H_{11}Cl_2NO_2$		3-(3,5-dichlorophenyl)-1,5-dimethyl-3-azabicyclo[3.1.0]hexanedione					
	438.2	30.09	0	68.67	66.1	30.09	29.0
		2*A14+A128+2*A17+3*A12+2*A22*C22+2*A1					[221]
$C_{14}H_{11}NO_3$		N-salicylidene-*m*-aminobenzoic acid					
	464	33.11	0	71.36	77.9	33.11	36.2
		8*A10+4*A12+A36*C36+A31+A42+A6*B6					[216]
$C_{14}H_{12}$		9,10-dihydrophenanthrene					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
	306.5	12.8	0	41.77	54.7	12.8	16.8
		8*A10+A14+3*A15+4*A19					[216]
$C_{14}H_{12}$		*trans*-stilbene					
	398.2	27.4	0	68.81	69.7	27.4	27.8
		10*A10+2*A12+2*A6					[215]
$C_{14}H_{12}$		9-methylfluorene					
	319.2	16.32	0	51.13	53.9	16.32	17.2
		A14+2*A15+4*A19+A16+A1+8*A10					[252]
$C_{14}H_{12}F_3NO_4S_2$		1,1,1-trifluoro-*n*-[2-methyl-4-(phenylsulphonyl)phenyl]methane sulfonamide					
	418.4	31.79	0	75.97	68.7	31.79	36.0
		8*A10+A11+3*A12+A88+A95+A4*B4+3*A25+A1					[221]
$C_{14}H_{12}O_2$		diphenylacetic acid					
	420.4	31.25	0	74.34	58.7	31.25	24.7
		10*A10+2*A11+A3*B3+A36					[216]
$C_{14}H_{12}O_2$		benzyl benzoate					
	293.1	20.44	0	69.76	71.9	20.44	21.1
		10*A10+A11+A12+A2+A38					[221]
$C_{14}H_{12}O_4$		1,2-dicarbomethoxynaphthalene					
	358.2	27.6	0	77.05	65.1	27.6	23.3
		6*A10+4*A12+2*A1+2*A38					[217]
$C_{14}H_{12}O_4$		1,3-dicarbomethoxynaphthalene					
	378.7	30.5	0	80.54	65.1	30.5	24.64
		6*A10+2*A12+2*A1+2*A38+2*A12					[217]
$C_{14}H_{12}O_4$		1,4-dicarbomethoxynaphthalene					
	340.2	20.4	0	59.96	65.1	20.4	22.13
		6*A10+2*A12+2*A1+2*A38+2*A12					[217]
$C_{14}H_{12}O_4$		1,5-dicarbomethoxynaphthalene					
	392	26.4	0	67.35	65.1	26.4	25.5
		6*A10+2*A12+2*A1+2*A38+2*A12					[217]
$C_{14}H_{12}O_4$		1,6-dicarbomethoxynaphthalene					
	371.8	22.1	0	59.44	65.1	22.1	24.2
		6*A10+2*A12+2*A1+2*A38+2*A12					[217]
$C_{14}H_{12}O_4$		1,7-dicarbomethoxynaphthalene					
	363.2	20	0	55.07	65.1	20	23.6
		6*A10+2*A12+2*A1+2*A38+2*A12					[217]
$C_{14}H_{12}O_4$		2,3-dicarbomethoxynaphthalene					
	324.2	20.2	0	62.31	65.1	20.2	21.1
		6*A10+2*A12+2*A1+2*A38+2*A12					[217]
$C_{14}H_{12}O_4$		2,7-dicarbomethoxynaphthalene					
	410.2	26.6	0	64.85	65.1	26.6	26.7
		6*A10+2*A12+2*A1+2*A38+2*A12					[217]
$C_{14}H_{14}$		1,2,3,4-tetrahydrophenanthrene					
	302.6	11.17	36.91				
	285	5.83	20.44				
	298	1.77	5.92	63.28	49.5	18.76	14.7
		A14+3*A15+2*A19+2*A12+6*A10					[31]
$C_{14}H_{14}$		phenyl-*o*-tolylmethane					
	279.8	19.24	0	68.78	62.6	19.24	17.5
		9*A10+3*A11+A1+A2					[216]
$C_{14}H_{14}$*		2,2′-dimethylbiphenyl					
	293.1	2.28	0	7.78	0	2.28	0
		Prediction not made					[216]
$C_{14}H_{14}$		1,2-diphenylethane					
	273.2	2.25	8.23				
	324.3	22.73	70.09	78.32	69.2	24.98	22.4
		10*A10+2*A11+2*A2					[216]
$C_{14}H_{14}$*		2-ethylbiphenyl					
	267.1	2.07	0	7.74	0	2.07	0
		Prediction not made					[216]
$C_{14}H_{14}$		1,2,3,4-tetrahydroanthracene					
	373.3	19.16	51.33				
	388	2.92	7.53	58.85	49.5	22.08	19.2
		A14+3*A15+2*A19+6*A10+2*A12					[216]
$C_{14}H_{14}Cl_2N_2O$		1-[2-(2,4-dichlorophenyl)-2-(propenyloxy)ethyl]-1H-imidazole					
	322.6	30.5	0	94.55	74.5	30.5	24.0
		A14+2*A15+3*A18*B18+A119+A118+2*A2+A3*B3+A5+A6					[221]
		+3*A10+2*A12+A11+2*A22*E22+A32					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{14}H_{14}NO_4PS$		O-ethyl O-(4-nitrophenyl)phenylphosphonothioate					
	308.2	25.05	0	81.28	74.2	25.05	22.9
		9*A10+3*A12+A1+A2+A81					[221]
$C_{14}H_{14}O_2$		(*dl*) 1,2-diphenyl-1,2-dihydroxyethane					
	393	31.38	0	79.85	71.9	31.38	28.2
		10*A10+2*A11+2*A3*B3+2*A30*B30					[273]
$C_{14}H_{14}O_2$		(*d*) 1,2-diphenyl-1,2-dihydroxyethane					
	420.5	34.31	0	81.59	71.9	34.31	30.2
		10*A10+2*A11+2*A3*B3+2*A30*B30					[273]
$C_{14}H_{14}O_3$		2-(6-methoxy-2-naphthyl)propionic acid					
	439.2	29.41	0	66.96	58.6	29.41	25.7
		6*A10+3*A12+A11+2*A1+A3*B3+A36*B36+A32					[33]
$C_{14}H_{14}O_3$		2-pivaloylindan-1,3-dione					
	381.5	25.99	0	68.12	62.9	25.99	24.0
		A14+2*A15+2*A19+2*A114+4*A10+3*A1+A4*B4+A35+A16					[215]
$C_{14}H_{15}N_3$		N,N-dimethyl-4-phenylazoaniline					
	389.2	23.08	0	59.3	53.7	23.08	20.9
		2*A1+A43+9*A10+3*A12+2*A42					[13]
$C_{14}H_{16}$		heptacyclo[6.6.0[2,6].0[3,13].0[4,11].0[5.9].0[8,1].O[10.14]]tetradecane					
	355	14.67	41.32				
	440	5.57	12.66	53.98	31.0	20.24	13.6
		7*A14−7*A15+12*A16					[127]
$C_{14}H_{16}ClN_3O_2$		1-(4-chlorophenoxy)-3,3-dimethyl-(1H,1,2,4-triazol-1-yl)-2-butanone					
	351.4	22.87	0	65.06	76.6	22.87	26.9
		4*A10+2*A12+3*A1+A4*B4+A3*B3+A14+2*A15+2*A18*B18					[221]
		+2*A118+A22*F22+A119+A35+A32					
$C_{14}H_{16}F_3N_3O_4$		N-(cyclopropylmethyl)-2,6-dinitro-*n*-propyl-4-(trifluoromethyl)benzenamine					
	305.8	22.51	0	73.61	70.9	22.51	21.7
		3*A12+2*A10+A11+A4*B4+3*A25+2*A50+A43+A1+3*A2+A14+A16					[221]
$C_{14}H_{16}O_8$		1,2,3,4-tetracarbomethoxybenzene					
	404.7	40.4	0	99.79	85.9	40.4	34.8
		4*A1+4*A38+4*A12+2*A10					[217]
$C_{14}H_{16}O_8$		1,2,3,5-tetracarbomethoxybenzene					
	389.2	32.6	0	83.89	85.9	32.6	33.4
		4*A1+4*A38+4*A12+2*A10					[217]
$C_{14}H_{16}O_8$		1,2,4,5-tetracarbomethoxybenzene					
	416.7	35.7	0	85.4	85.9	35.7	35.8
		4*A1+4*A38+4*A12+2*A10					[217]
$C_{14}H_{17}ClNPO_4S_2$		S-[2-chloro-1-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]O,O-diethylphosphorodithioate					
	340.0	25.27	0	74.33	101.1	25.27	34.4
		A14+2*A15+2*A19+4*A10+A128+4*A2+2*A1+A80					[221]
$C_{14}H_{17}NO_2$		4-methyl-7-diethylaminocoumarin					
	343.8	17.88	0	52.02	67.2	17.88	23.1
		A14+3*A15+2*A19+A19+A18*B18+A115+3*A10+A12+3*A1+2*A2+A43					[216]
$C_{14}H_{18}$		1,2,3,4,5,6,7,8-octahydroanthracene					
	331.4	2.51	7.59				
	345.4	18.34	53.1	60.69	54.7	20.86	18.9
		2*A14+6*A15+4*A19+2*A10					[216]
$C_{14}H_{18}ClN_3O_2$		β(4-chlorophenoxy)-α-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol					
	377.8	24.47	0	64.77	73.0	24.47	27.6
		A14+2*A15+2*A118+A119+2*A18*B18+2*A3*B3					[221]
		+A32+A22*F22+4*A10+2*A12+3*A1+A4+A30*F30					
$C_{14}H_{19}Cl_2NO_2$		4[*p*-[bis(2-chloroethyl)amino]benzene]butanoic acid					
	338.9	29.18	0	86.1	102.7	29.18	34.8
		3*A2+4*A2+4*A10+A11+A12+A36*D36+2*A22*D22+A4					[221]
$C_{14}H_{19}NO$		2-(dimethylamino)-1,2-diphenylethanone					
	334.2	22.38	0	66.97	64.7	22.38	21.6
		10*A10+A11+A12+A35*B35+A43+2*A1+A3*B3					[253]
$C_{14}H_{20}$		diamantane					
	407.2	4.44	10.89				
	440.4	8.95	20.33				
	517.9	8.66	16.72	47.95	45.4	22.05	23.5
		5*A14−A15+8*A16					[216]
$C_{14}H_{20}$		1,8-cyclotetradecadiyne					
	370	22.6	0	61.06	55.3	22.6	20.4
		A14+11*A15+4*A20					[108]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{14}H_{20}O$		1-diamantanol					
	408	4.9	12.01				
	395	18	45.57				
	573	9.6	16.75	74.33	27.3	32.5	15.6
		$5*A14-A15+7*A16+A17+A30$					[144]
$C_{14}H_{20}O$		4-diamantanol					
	448	9.77	21.81				
	484	16.4	33.88	55.69	27.3	26.17	13.2
		$5*A14-A15+7*A16+A17+A30$					[144]
$C_{14}H_{20}ClNO_2$		2-chloro-N-(2,6-diethylphenyl)-N-(methoxymethyl)acetamide					
	315.9	25.31	0	80.13	86.5	25.31	27.3
		$3*A1+4*A2+3*A10+2*A11+A12+A32+A22*C22+A59$					[221]
$C_{14}H_{20}N_3O_5PS$		O-6-ethoxycarbonyl-5-methylpyrazolo[1,5-*a*]pyrimidin-2-yl O,O-diethyl phosphorothioate					
	324.4	27.32	0	84.22	97.6	27.32	31.66
		$A14+2*A15+A18+2*A19+A118+A119+A10+A11+A12+A41+A38+4*A1+3*A2+A79$					[221]
$C_{14}H_{21}N_3O_4$		4-(1,1-dimethylethyl)-*n*-(1-methylpropyl)-2,6-dinitrobenzeneamine					
	338.8	20.84	0	61.52	63.5	20.84	21.5
		$2*A10+A11+3*A12+5*A1+A4+A2+A3*B3+2*A50+A44$					[221]
$C_{14}H_{22}$		*n*-octylbenzene					
	234.2	29.96	0	127.91	110.4	29.96	25.9
		$A1+7*A2*B2+5*A10+A11$					[216]
$C_{14}H_{22}N_4O_2$		8-heptyltheophylline					
	472.7	33	0	69.81	95.9	33	45.3
		$2*A14+3*A15+2*A125+A118+A121+3*A1+3*A1+3*A19+6*A2$					[216]
$C_{14}H_{22}N_4O_6S$		4-(dipropylamino)-N,N-dimethyl-3,5-dinitrobenzenesulfonamide					
	413.6	32.57	0	78.75	85.7	32.57	35.4
		$4*A1+4*A2+A43+2*A50+A94+2*A10+4*A12$					[221]
$C_{14}H_{22}O$		2,6-di-*tert*-butylphenol					
	310.7	16.57	0	53.33	51.6	16.57	16.0
		$6*A1+2*A4+2*A11+A12+3*A10+A31$					[101]
$C_{14}H_{24}$		1,3,5,7-tetramethyladamantane					
	183.3	0.23	1.25				
	337.2	9.82	29.12	30.38	35.9	10.05	12.1
		$3*A14+A15+4*A17+4*A1$					[146]
$C_{14}H_{24}$		*cis*-anti-*trans*-perhydrophenanthrene					
	313	11.16	0	35.64	59.7	11.16	18.7
		$3*A14+5*A15+4*A16$					[216]
$C_{14}H_{24}$		*cis*-syn-*trans*-perhydrophenanthrene					
	273	10.48	0	38.39	59.7	10.48	16.3
		$3*A14+5*A15+4*A16$					[216]
$C_{14}H_{24}$		*trans*-anti-*trans*-perhydrophenanthrene					
	283	11.83	0	41.81	59.7	11.83	16.9
		$3*A14+5*A15+4*A16$					[216]
$C_{14}H_{24}O_2$		1,8-cyclotetradecanedione					
	417.2	27.53	0	65.99	71.4	27.53	29.8
		$A14+11*A15+2*A114$					[114]
$C_{14}H_{24}NO_4PS_3$		O,O-diisopropyl S-2-phenylsulfonylaminoethyl phosphorodithioate					
	310.4	30.61	0	98.63	91.2	30.61	28.3
		$5*A10+A12+2*A2+4*A1+2*A3*B3+A95+A80$					[221]
$C_{14}H_{24}O_4$		1,6-cyclodecanedione bis ethylene ketal					
	450.2	32.68	0	72.58	69.2	32.68	31.2
		$3*A14+9*A15+4*A112+2*A17$					[114]
$C_{14}H_{26}O$		4,4,8,8-tetramethylcyclodecanone					
	378.2	16.32	0	43.15	59.1	16.32	22.4
		$A14+7*A15+4*A1+2*A17+A114$					[111]
$C_{14}H_{26}O_2$		decyl methacrylate					
	250.7	30.55	0	121.85	133.4	30.55	33.5
		$2*A1+9*A2*B2+A5+A7+A38$					[216]
$C_{14}H_{28}$		cyclotetradecane					
	328	28.7	0	87.51	74.1	28.7	24.3
		$11*A15+A14$					[119]
$C_{14}H_{28}O$		2-tetradecanone					
	306.7	49.12	0	160.16	142.4	49.12	43.7
		$2*A1+A35+11*A2*B2$					[216]
$C_{14}H_{28}O_2$		ethyl dodecanoate					
	271.5	9.31	0	34.3	0	9.31	
		Prediction not made					[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
$C_{14}H_{28}O_2$		tetradecanoic acid					
	327	45.1	0	137.92	142.9	45.1	46.7
		12*A2*B2+A1+A36					[216]
$C_{14}H_{28}O_4$		2,2,9,9-tetramethyl-1,3,8,10-tetraoxacyclotetradecane					
	409.4	30.5	0	74.5	80.1	30.5	32.8
		A14+11*A15+4*A112+4*A1+2*A17					[27]
$C_{14}H_{29}NO_3$		N-dodecylglycine					
	393.1	48.4	0	123.12	138.2	48.4	54.3
		A1+11*A2*B2+A2+A36*B36+A44					[249]
$C_{14}H_{29}NO_3$		N-octyl-L-leucine					
	357.1	7.6	21.28				
	398.1	29.3	73.6	94.88	110.0	36.9	43.8
		3*A1+7*A2*B2+A3+A3*B3+A36*B36+A44+A2					[249]
$C_{14}H_{29}NO_3$		N-octyl-DL-leucine					
	353.6	6.8	19.23				
	367.1	27.2	74.09	93.33	110.0	34.0	40.4
		3*A1+7*A2*B2+A3+A3*B3+A36*B36+A44+A2					[249]
$C_{14}H_{30}$		tetradecane					
	279	45.07	0	161.54	147.1	45.07	41.1
		2*A1+12*A2*B2					[216]
$C_{14}H_{30}O$		1-tetradecanol					
	311.2	47.01	151.04				
	310.8	25.1	80.75				
	306	1.8	5.86				
	311	23.81	76.57				
	311.6	22.01	70.71				
	311	49.37	158.75	158.75	140.6	49.37	43.7
		A1+13*A2*B2+A30					[224]
$C_{14}H_{30}O_2S$		3(*n*-undecylthio)-1,2-propanediol					
	280.2	2.5	8.92				
	289.1	4.9	16.95				
	295.2	4.6	15.58				
	317.4	18.3	57.66	99.11	151.6	30.3	48.1
		A1+10*A2*B2+A84+2*A30*C30+2*A2+A3*B3					[217]
$C_{14}H_{30}O_3$		3(*n*-undecyloxy)-1,2-propanediol					
	311.7	43.1	0	138.27	154.2	43.1	48.1
		A1+10*A2*B2+A32+2*A30*C30+2*A2+A3*B3					[217]
$C_{14}H_{31}NO_2$		3(*n*-undecylamino)-1,2-propanediol					
	348.8	58.2	0	166.86	144.2	58.2	50.3
		A1+10*A2*B2+A44+2*A30*C30+2*A2+A3*B3					[217]
$C_{15}H_{10}N_2O_2$		4,4′-diphenylmethane diisocyanate					
	313.6	27.3	0	87.06	78.5	27.3	24.6
		8*A10+2*A12+2*A11+2*A58+A2					[216, 104]
$C_{15}H_{11}ClF_3NO_4$		2-chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene					
	358.8	30.07	0	83.8	82.4	30.07	29.6
		6*A10+A11+5*A12+A1+A2+A4*B4+3*A25+A22*G22+A50+2*A32					[215]
$C_{15}H_{11}ClN_2O$		7-chloro-1,3-dihydro-5-phenyl-2H-1,4-benzodiazepin-2-one					
	216.7	34	0	156.9	69.7	34	15.1
		A14+4*A15+2*A121+A22*C22+A16+A19+A18+5*A10+A12					[216]
$C_{15}H_{12}$		4-methylphenanthrene					
	182	0.02	0.12				
	295	0.03	0.11				
	324.9	14.04	43.21	43.44	44.8	14.09	14.6
		A1+9*A10+4*A12+A11					[216]
$C_{15}H_{12}N_2O_3$		1,4-diamino-2-methoxyanthraquinone					
	515.2	35.29	0	68.5	72.4	32.29	37.3
		A14+3*A15+2*A114+4*A19+5*A10+2*A45+3*A12+A1+A32					[13]
$C_{15}H_{13}Cl_2NO_2$		1,1-(di-*p*-chlorophenyl)-2-nitropropane					
	354.3	21.39	0	60.38	66.8	21.39	23.7
		8*A10+2*A11+2*A12+A3+A3*B3+A1+2*A22*C22+A50					[221]
$C_{15}H_{14}O$		1,3-diphenylacetone					
	307.2	20.2	0	65.77	73.8	20.2	22.7
		10*A10+2*A11+2*A2+A35					[217]
$C_{15}H_{15}ClN_2O_2$		3-[4-[4-chlorophenoxy]phenyl]-1,1-dimethylurea					
	425.8	34.87	0	81.88	82.9	34.87	35.3
		8*A10+4*A12+2*A1+A22*C22+A32*C32+A64*B64					[215]
$C_{15}H_{15}N$		N-isopropylcarbazole					
	137.5	0.64	4.64				
	180	0.38	2.09				

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
	395.2	17.73	44.86	51.6	57.2	18.75	22.6
		$A14+2*A15+2*A19+8*A10+2*A1+A3*B3+A119+2*A19$					[142]
$C_{15}H_{15}NO$		N-methyldiphenylacetamide					
	439.8	30.23	0	68.73	64.3	30.23	28.3
		$10*A10+2*A11+A3*B3+A1+A60$					[221]
$C_{15}H_{16}N_2O_2$		*a*-cyclopropyl-*a*-(4-methoxyphenyl)-5-pyrimidinemethanol					
	383.1	26.63	0	69.51	88.0	26.63	33.7
		$A14+7*A10+A1+A4*B4+2*A11+A12+2*A41+A30*D30+A32+A16$					[221]
$C_{15}H_{16}O$		*p*-α-cumylphenol					
	346.4	21.68	0	62.58	66.3	21.68	23.0
		$8*A10+3*A12+A11+2*A1+A3+A31$					[216]
$C_{15}H_{16}O_2$		4,4′dihydroxydiphenyl-2,2-propane					
	433	30.1	0	69.52	66.0	30.1	28.6
		$2*A1+A4+8*A10+2*A12+2*A11+2*A31$					[216]
$C_{15}H_{17}Br_2NO_2$		3,5-dibromo-4-hydroxybenzonitrile octanoyl ester					
	318.3	26.49	0	83.23	105.8	26.49	33.7
		$4*A12+2*A10+2*A21+A56+A38+A1+6*A2$					[221]
$C_{15}H_{18}Cl_2N_2O_3$		3-[2,4-dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2(3H)-one					
	360.6	26.39	0	73.19	89.3	26.39	32.2
		$A14+2*A15+A19+A126+A118+5*A1+A3*B3+A4+4*A12+2*A10+2*A22*E22+A32$					[221]
$C_{15}H_{18}N_2O_6$		2-sec-butyl-4,6-dinitrophenyl 3-methylcrotonate					
	341.3	18.89	0	55.37	80.2	18.89	27.4
		$4*A1+A2+A3+2*A10+3*A12+A11+2*A50+A38+A7+A6*B6$					[222]
$C_{15}H_{21}NO$		2-methyl-1-phenyl-2-(N-piperidinyl)-1-propanone					
	310.2	16.74	0	53.97	71.7	16.74	22.2
		$5*A10+A12+A4*B4+2*A1+A14+3*A15+A119+A35$					[254]
$C_{15}H_{21}NO_4$		methyl N-(2-methoxyacetyl)-N-(2,6̄-xylyl)-dl-alaninate					
	345.5	26.46	0	76.58	82.1	26.46	28.4
		$5*A1+A2+A3*B3+3*A10+2*A11+A12+A38+A32+A59$					[221]
$C_{15}H_{23}N_3O_2$		N-capryl-pyrazinamide					
	360.5	50.58	0	140.31	104.7	50.58	37.7
		$A1+6*A2+3*A10+A12+2*A41+A71$					[9]
$C_{15}H_{24}O$		2,6-di-*tert*-butyl-4-methylphenol					
	343.7	23.85	0	69.39	52.2	23.85	17.9
		$7*A1+2*A10+3*A11+A12+2*A4+A31$					[101]
$C_{15}H_{24}O_2$		2,6-di-*tert*-butyl-4-methoxyphenol					
	374.4	26.9	0	71.86	59.0	26.9	22.1
		$7*A1+2*A4+2*A11+2*A12+2*A10+A31+A32$					[114]
$C_{15}H_{28}O_2$		pentadecanolactone					
	283	27.3	96.47				
	308.5	6.99	22.65	119.12	84.6	34.29	26.1
		$A14+13*A15+A115$					[282]
$C_{15}H_{30}$		cyclopentadecane					
	210.1	8.5	40.46				
	336.6	8.5	25.25	65.71	77.8	17	26.2
		$A14+12*A15$					[181]
$C_{15}H_{30}$		*n*-decylcyclopentane					
	251.0	33.14	0	132.01	127.6	33.14	32.0
		$A14+A16+A1+9*A2*B2+2*A15$					[216]
$C_{15}H_{30}O$		2-pentadecanone					
	312.2	54.57	0	174.8	151.7	54.39	47.4
		$2*A1+A35+12*A2*B2$					[216]
$C_{15}H_{30}O_2$		pentadecanoic acid					
	318.7	8.12	25.48				
	325.7	41.52	127.49	152.97	152.3	49.64	49.6
		$13*A2*B2+A1+A36$					[216]
$C_{15}H_{30}O_2$		methyl myristate					
	291.6	50.21	0	172.17	154.8	50.21	45.1
		$2*A1+12*A2*B2+A38$					[217]
$C_{15}H_{31}NO_3$		N-decyl-L-valine					
	378.1	21.3	56.33				
	380.6	15.4	40.46	96.8	121.5	36.7	46.3
		$3*A1+A3+A3*B3+9*A2*B2+A44+A36*B36$					[249]
$C_{15}H_{31}NO_3$		N-decyl-DL-valine					
	358.1	63.1	0	176.21	121.5	63.1	43.5

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
		3*A1+A3+A3*B3+9*A2*B2+A44+A36*B36					
$C_{15}H_{31}NO_3$		N-dodecyl-L-alanine					[249]
	356.1	37.6	0	105.59	139.0	37.6	49.5
		2*A1+11*A2*B2+A3*B3+A36*B36+A44					[249]
$C_{15}H_{32}$		*n*-pentadecane					
	270.9	9.17	33.85				
	283.1	34.6	122.17	156.02	156.5	43.77	44.3
		2*A1+13*A2*B2					[216]
$C_{15}H_{32}O$		1-pentadecanol					
	316	23.64	74.81				
	316.6	54.73	172.86	172.8	150.0	54.73	47.5
		A1+14*A2*B2+A30					[224]
$C_{15}H_{32}O_2S$		3(*n*-dodecylthio)-1,2-propanediol					
	299	18.1	60.54				
	325.5	20.3	62.37	122.9	160.9	38.4	52.4
		A1+11*A2*B2+A84+2*A30*C30+2*A2+A3*B3					[217]
$C_{15}H_{32}O_3$		3(*n*-dodecyloxy)-1,2-propanediol					
	323	51.4	0	159.13	163.5	51.4	52.8
		A1+11*A2*B2+A32+2*A30*C30+2*A2+A3*B3					[217]
$C_{15}H_{33}NO_2$		3(*n*-dodecylamino)-1,2-propanediol					
	351.9	62.1	0	176.47	153.5	62.1	54.0
		A1+11*A2*B2+A44+2*A30*C30+2*A2+A3*B3					[217]
$C_{16}F_{34}$		perfluorohexadecane					
	176.5	1.13	6.4				
	177.7	3.01	16.94				
	186.7	1.89	10.12				
	402.2	61.09	151.89	185.35	172.0	67.12	69.2
		16*A4*B4+6*A25+28*A26					[67]
$C_{16}H_{10}$		pyrene					
	120.8	0.29	2.39				
	423.8	17.36	40.97	43.36	43.8	17.65	18.6
		10*A10+4*A12+2*A13					[216]
$C_{16}H_{10}$		1,2-benzacenaphthene (fluoranthene)					
	383.4	18.74	0	48.89	36.5	18.74	14.0
		10*A10+5*A12+A13					[216]
$C_{16}H_{11}F_3O$		4-ethoxy-2′,3′,4′-trifluorodiphenylacetylene					
	356.8	32.2	0	90.25	73.4	32.2	26.2
		6*A10+6*A12+2*A9+A2+A1+3*A24+A32					[196]
$C_{16}H_{12}F_2$		4-ethyl-3′,4′-difluorodiphenylacetylene					
	301.2	16.6	0	55.11	64.8	16.6	19.5
		7*A10+A11+4*A12+2*A9+A2+A1+2*A24					[196]
$C_{16}H_{12}F_2O$		4-ethoxy-2′,4′-difluorodiphenylacetylene					
	343.4	27	0	78.63	71.64	27	24.6
		7*A10+5*A12+2*A9+A2+A1+2*A24+A32*C32					[196]
$C_{16}H_{13}FO$		4-ethoxy-4′-fluorodiphenylacetylene					
	354.4	22.8	0	64.33	69.9	22.8	24.8
		8*A10+4*A12+2*A9+A2+A1+A24*B24+A32					[196]
$C_{16}H_{12}Ge$		diphenyldiethynylgermane					
	320	20.1	0	62.81	48.3	20.1	15.5
		10*A10+2*A12+2*A8+2*A9+A102					[48]
$C_{16}H_{12}Si$		diphenyldiethynylsilane					
	316.2	19.67	0	62.21	52.2	19.67	16.5
		10*A10+2*A11+2*A8+2*A9+A109					[216]
$C_{16}H_{14}$		4,5,9,10-tetrahydropyrene					
	319.9	1.85	5.77				
	385.1	0.13	0.34				
	412.8	17.09	41.41	47.53	52.5	19.07	21.7
		2*A14+4*A15+6*A19+6*A10					[18]
$C_{16}H_{14}Cl_2O_3$		ethyl 2-hydroxy-2,2-bis-(4-chlorophenyl)acetate					
	310.4	23.48	0	75.64	90.0	23.48	27.9
		8*A10+2*A11+2*A12+A1+A2+A4*B4+2*A22*D22+A30*D30+A38					[215]
$C_{16}H_{14}Cl_2O_4$		methyl 2-(4-(2,4-dichlorophenoxy)phenoxy)propionate					
	314.4	27.08	0	86.13	89.3	27.08	28.1
		7*A10+5*A12+2*A1+A3*B3+A38+2*A32+2*A22*D22					[221]
$C_{16}H_{14}O_2$		1,2-dibenzoylethane					
	187	0.22	1.17				
	418.6	38.99	93.3	94.56	82.6	39.21	34.6
		10*A10+2*A12+2*A2+2*A35					[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{16}H_{14}O_6$		1,2,3-tricarbomethoxynaphthalene					
	362.7	23.7	0	65.34	75.4	23.7	27.4
		3*A1+3*A38+2*A12+5*A10+3*A12					[217]
$C_{16}H_{14}O_6$		1,2,4-tricarbomethoxynaphthalene					
	393.7	32.1	0	81.53	75.4	32.1	29.7
		3*A1+3*A38+2*A12+5*A10+3*A12					[217]
$C_{16}H_{14}O_6$		1,2,5-tricarbomethoxynaphthalene					
	363	25.5	0	70.25	75.4	25.5	27.4
		3*A1+3*A38+2*A12+5*A10+3*A12					[217]
$C_{16}H_{14}O_6$		1,2,6-tricarbomethoxynaphthalene					
	416.7	35.9	0	86.15	75.4	35.9	31.4
		3*A1+3*A38+2*A12+5*A10+3*A12					[217]
$C_{16}H_{14}O_6$		1,2,7-tricarbomethoxynaphthalene					
	427.2	36.1	0	84.5	75.4	36.1	32.2
		3*A1+3*A38+2*A12+5*A10+3*A12					[217]
$C_{16}H_{14}O_6$		1,2,8-tricarbomethoxynaphthalene					
	366.7	24.8	0	67.63	75.4	24.8	27.7
		3*A1+3*A38+2*A12+5*A10+3*A12					[217]
$C_{16}H_{14}O_6$		1,3,5-tricarbomethoxynaphthalene					
	402.7	25.9	0	64.35	75.4	25.9	30.4
		3*A1+3*A38+2*A12+5*A10+3*A12					[217]
$C_{16}H_{14}O_6$		1,3,7-tricarbomethoxynaphthalene					
	446.7	37.2	0	83.39	75.4	37.2	33.7
		3*A1+3*A38+2*A12+5*A10+3*A12					[217]
$C_{16}H_{14}O_6$		1,3,8-tricarbomethoxynaphthalene					
	388.2	27.7	0	71.46	75.4	27.7	29.3
		3*A1+3*A38+2*A12+5*A10+3*A12					[217]
$C_{16}H_{14}O_6$		1,4,5--tricarbomethoxynaphthalene					
	402.2	26.5	0	65.77	75.4	26.5	30.3
		3*A1+3*A38+2*A12+5*A10+3*A12					[217]
$C_{16}H_{14}O_6$		1,4,6-tricarbomethoxynaphthalene					
	409.2	30.2	0	73.6	75.4	30.2	30.9
		3*A1+3*A38+2*A12+5*A10+3*A12					[217]
$C_{16}H_{14}O_6$		2,3,5-tricarbomethoxynaphthalene					
	401.7	41	0	101.96	75.4	41	30.3
		3*A1+3*A38+2*A12+5*A10+3*A12					[217]
$C_{16}H_{14}O_6$		2,3,6-tricarbomethoxynaphthalene					
	399.2	34.4	0	86.27	75.4	34.4	30.1
		3*A1+3*A38+2*A12+5*A10+3*A12					[217]
$C_{16}H_{15}Cl_2NO_2$		1,1-bis(4-chlorophenyl)-2-nitrobutane					
	330.3	15.41	0	46.65	73.8	15.41	24.4
		8*A10+2*A12+2*A11+A3+A3*B3+A1+A2+2*A22*C22+A50					[221]
$C_{16}H_{15}Cl_3O_2$		1-methoxy-2-(2,2,2-trichloro-1(4-methoxyphenyl)ethyl)benzene					
	347.6	22.45	0	64.58	85.6	22.45	29.8
		8*A10+2*A12+2*A11+2*A1+A4*B4+2*A32+3*A22*E22+A3*B3					[221]
$C_{16}H_{15}Cl_3O_2$		1,1′-(2,2,2-trichloroethylidene-bis(4-methoxy)benzene					
	360.6	27.48	76.14	76.21	85.6	27.48	30.9
		8*A10+2*A12+2*A11+2*A1+A4*B4+2*A32+3*A22*E22+A3*B3					[221]
$C_{16}H_{15}N$		4′-propylbiphenyl-4-carbonitrile					
	338.8	22.7	0	67.01	76.8	22.7	26.0
		A1+2*A2+8*A10+A11+3*A12+A56					[216]
$C_{16}H_{16}$		1,2,3,6,7,8-hexahydropyrene					
	377	5.02	13.32				
	407.7	18.09	44.37	57.69	45.0	23.11	18.4
		2*A14+6*A15+6*A19+4*A10					[18]
$C_{16}H_{16}N_2O_2$*		anisaldazine					
	442	29.75	0	67.31	0	29.75	0
		No prediction made					[216]
$C_{16}H_{16}N_2O_4$		ethyl [3-[[(phenylamino)carbonyl]oxy]phenylcarbamate					
	394.1	32.75	0	83.09	90.2	32.75	35.6
		9*A10+3*A12+2*A69+A1+A2					[221]
$C_{16}H_{16}N_2O_4$		methyl 3-*m*-tolylcarbamoyloxphenylcarbamate					
	423.8	39.62	0	93.49	83.6	39.62	35.4
		2*A1+3*A12+A11+8*A10+2*A69					[221]
$C_{16}H_{16}O_2$		(*d*) 2-(*p*-methoxyphenyl)propiophenone					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
	326	21.76	0	66.74	76.8	21.76	25.0
		9*A10+2*A12+A3*B3+2*A1+A32+A11+A35					[273]
$C_{16}H_{16}O_2$		(*dl*) 2-(*p*-methoxyphenyl)propiophenone					
	353	26.36	0	74.67	76.8	26.36	27.1
		9*A10+2*A12+A3*B3+2*A1+A32+A11+A35					[273]
$C_{16}H_{16}O_3$		2,2-dimethoxy-1,2-diphenylethanone					
	338.5	20.86	0	61.63	83.4	20.86	28.2
		10*A10+A11+A12+2*A1+2*A32*C32+A35+A4*B4					[28]
$C_{16}H_{17}NO$		N,N-dimethyl-2,2-diphenylacetamide					
	407.1	25.43	67.55	62.47	69.3	25.43	28.2
		2*A1+10*A10+2*A11+A3*B3+A59					[217]
$C_{16}H_{18}FN_3O_3$		1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylic acid					
	500.2	32.97	0	65.91	82.5	32.97	41.3
		2*A14+6*A15+2*A119+A121+A114+3*A19					[36]
		+A18*B18+2*A12+2*A10+A24+A36+A1+A2					
$C_{16}H_{18}N_2O$*		4-*n*-butyl-4′-hydroxyazobenzene					
	351.6	5.25	0	14.93	0	5.25	0
		No prediction made					[131]
$C_{16}H_{18}N_4O_4$		N,N-(2-hydroxyethyl)-4-(4-nitrophenyl)azoaniline					
	484.2	32.43	0	66.97	92.1	32.43	44.6
		8*A10+4*A12+4*A2+2*A30*+E30*+2*A42+A43+A50					[13]
$C_{16}H_{19}BrO_2$		4-*trans*-(4-bromophenyl)cyclohexyl (E)-2-butenoate					
	388.2	28.4	0	73.16	79.6	28.4	30.9
		A14+3*A15+2*A16+4*A10+A11+A12+A21+A38					[140]
		+A1+A6*B6+A6					
$C_{16}H_{19}ClO_2$		4-*trans*-(4-chlorophenyl)cyclohexyl (E)-2-butenoate					
	386.2	30.2	0	78.2	78.2	30.2	30.2
		A14+3*A15+2*A16+4*A10+A11+A12+A38					[140]
		+A1+A6*B6+A6+A22*B22					
$C_{16}H_{19}FO_2$		4-*trans*-(4-fluorophenyl)cyclohexyl (E)-2-butenoate					
	354.2	25.1	0	70.86	78.6	25.1	27.9
		A14+3*A15+2*A16+4*A10+A11+A12+A38+A1+A6*B6+A6+A24					[140]
$C_{16}H_{19}N_3O_2$		N,N-(2-hydroxyethyl)-4-phenylazoaniline					
	407	29.96	0	73.61	89.3	29.96	36.3
		9*A10+3*A12+4*A2+2*A30*E30+2*A42+A43					[13]
$C_{16}H_{20}N_2$		tetracyclopropylsuccinonitrile					
	390	22.3	0	57.18	64.4	22.3	25.1
		4*A14+4*A16+2*A4*B4+2*A56					[216]
$C_{16}H_{20}O_6P_2S_3$		O,O,O′,O′-tetramethyl O,O′-thiodi-*p*-phenylene bis(phosphorothioate)					
	303.2	33.03	0	108.94	104.0	33.03	31.5
		8*A10+4*A12+A84+2*A79+4*A1					[221]
$C_{16}H_{22}NClO_3$		N-(chloroacetyl)-*n*-(2,6-diethylphenyl)glycine ethyl ester					
	318	23.84	0	74.97	96.6	23.84	30.7
		3*A1+5*A2+3*A10+2*A11+A12+A22*C22+A59+A38					[221]
$C_{16}H_{22}O_3Si_3$		1,1,3,3-tetramethyl-5,5-diphenylcyclotrisiloxane					
	338.0	22.19	0	65.66	69.3	22.19	23.4
		4*A1+A14+3*A15+3*A112+3*A139+10*A10+2*A11					[216]
$C_{16}H_{24}N_6$		1-(methylphenethylamino)-3,5-bis(dimethylamino)-*s*-triazine					
	334.2	20.04	0	59.96	73.2	20.04	24.5
		5*A1+2*A2+A11+5*A10+3*A41+3*A12+3*A43					[215]
$C_{16}H_{25}NO_2$		nonyl phenylcarbamate					
	327	28.07	0	85.77	132.4	28.07	43.3
		5*A10+A12+A1+8*A2*B2+A69					[102]
$C_{16}H_{28}O_2$		1,9-cylohexadecanedione					
	301.2	17.95	59.59				
	351.2	8.03	22.87	82.47	78.8	25.98	27.7
		A14+13*A15+2*A114					[114]
$C_{16}H_{28}O_4$		1,7-cyclododecanedione bis ethylene ketal					
	478.2	36.94	0	77.26	76.6	36.94	36.6
		3*A14+11*A15+2*A17+4*A112					[114]
$C_{16}H_{32}$		cyclohexadecane					
	271.2	18.83	69.42				
	283.2	1.26	4.43				
	332.2	4.18	12.59	86.45	81.5	24.27	27.1
		A14+13*A15					[112]
$C_{16}H_{32}$		*n*-decylcyclohexane					
	271.4	38.62	0	142.29	131.3	38.62	35.6

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
		9*A2*B2+A1+A14+3*A15+A16					[215]
$C_{16}H_{32}$		1-hexadecene					
	249.2	3.87	15.53				
	277.5	30.21	108.86	124.39	161.5	34.08	44.8
		A5+A6+13*A2*B2+A1					[165]
$C_{16}H_{32}O_2$		hexadecanoic acid					
	335.7	54.81	0	163.27	161.6	54.81	54.2
		14*A2*B2+A1+A36					[216]
$C_{16}H_{32}O_4$		6,6,14,14-tetramethyl-1,3,9,11-tetraoxacyclohexadecane					
	358.6	29.71	0	82.84	87.5	29.71	31.4
		A14+13*A15+4*A112+4*A1+2*A17					[117]
$C_{16}H_{32}O_4$		2,2,10,10-tetramethyl-1,3,9,11-tetraoxacyclohexadecane					
	371.3	25.94	0	69.87	87.5	25.94	32.5
		A14+13*A15+4*A112+4*A1+2*A17					[117]
$C_{16}H_{32}O_8$		1,4,7,10,13,16,19,22-octaoxacyclotetracosane					
	292.2	34.5	0	118.07	118.4	34.5	34.6
		A14+21*A15+6*A112					[120]
$C_{16}H_{33}NO$		N-hexyl decanamide					
	301	6	19.93				
	311	31	99.68	119.61	157.9	37	49.1
		2*A1+13*A2*B2+A60					[127]
$C_{16}H_{33}NO$		N-butyl dodecanamide					
	322.1	39	0	121.08	151.0	39.0	48.7
		2*A1+10*A2*B2+A60+3*A2					[127]
$C_{16}H_{33}NO_3$		N-tetradecylglycine					
	379.6	6.8	17.91				
	396.6	47.4	119.52	137.43	156.8	54.2	62:2
		13*A2*B2+A1+A44+A36*B36+A2					[249]
$C_{16}H_{33}NO_3$		N-decyl-L-leucine					
	343.1	1.2	3.5				
	383.1	27.5	71.78	75.28	128.7	28.7	49.3
		3*A1+9*A2*B2+A3+A3*B3+A36*B36+A44+A2					[249]
$C_{16}H_{33}NO_3$		N-decyl-DL-leucine					
	357.1	28.9	0	71.78	128.7	28.9	45.9
		3*A1+9*A2*B2+A3+A3*B3+A36*B36+A44+A2					[249]
$C_{16}H_{34}$		hexadecane					
	291.3	53.35	183.13				
	291.1	51.46	176.79	176.79	165.8	53.35	48.3
		2*A1+14*A2*B2					[216]
$C_{16}H_{34}O$		1-hexadecanol					
	322.3	33.6	104.18				
	322.2	23.72	73.22				
	322.2	58.41	181.17	181.17	159.3	58.41	51.3
		A1+15*A2*B2+A30					[224]
$C_{16}H_{34}O_2S$		3(*n*-tridecylthio)-1,2-propanediol					
	296.9	11.3	38.06				
	330.6	22.7	68.66	106.72	170.3	34	56.3
		A1+12*A2*B2+A84+2*A30*C30+2*A2+A3*B3					[217]
$C_{16}H_{34}O_3$		3(*n*-tridecyloxy)1-2-propanediol					
	342.2	51.4	0	158.54	172.9	51.4	56.0
		A1+12*A2*B2+A32+2*A30*C30+2*A2+A3*B3					[217]
$C_{16}H_{35}NO_2$		3(*n*-tridecylamino)-1,2-propanediol					
	354.9	68.7	0	193.58	162.9	68.7	57.8
		A1+12*A2*B2+A44+2*A30*C30+2*A2+A3*B3					[217]
$C_{16}H_{36}Ge$		tetrabutylgermane					
	198.6	19.1	0	96.17	120.8	19.1	24.0
		4*A1+12*A2+A102					[53]
$C_{16}H_{40}O_4Si_4$		octaethylcyclotetrasiloxane					
	208.2	12.22	58.7				
	213.4	13.71	64.24	122.94	115.7	25.92	24.7
		8*A1+8*A2+4*A112+4*A139+A14+5*A15					[227]
$C_{17}H_{12}$		1,2-benzofluorene					
	399.9	3.8	9.5				
	462.8	18.4	39.76	49.26	50.9	22.2	23.6
		A14+2*A15+4*A19+10*A10+2*A12					[216]
$C_{17}H_{12}$		2,3-benzofluorene					
	489.7	23.4	0	47.78	50.9	23.4	24.9
		A14+2*A15+4*A19+10*A10+2*A12					[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{17}H_{12}O$		4-ethynyl-1-[(4-ethynylphenyl)methoxy]benzene					
	371.2	21.2	0	57.11	63.4	21.2	23.5
		2*A9+2*A8+3*A12+A11+A2+A32+8*A10					[216]
$C_{17}H_{12}O_2$		4-benzoyl-1-naphthol					
	440.6	28.64	0	65	69.0	28.64	30.4
		11*A10+5*A12+A35+A31					[215]
$C_{17}H_{12}O_2$		1-benzoyl-2-naphthol					
	414.1	31.35	0	75.71	69.0	31.35	28.6
		11*A10+5*A12+A35+A31					[215]
$C_{17}H_{12}O_2$		2-benzoyl-1-naphthol					
	343.9	20.18	0	58.68	69.0	20.18	23.7
		11*A10+5*A12+A35+A31					[215]
$C_{17}H_{12}O_2$		1-naphthyl benzoate					
	329.2	16.98	0	51.58	66.7	16.98	22.0
		12*A10+4*A12+A38					[118]
$C_{17}H_{12}O_2$		2-naphthyl benzoate					
	381.2	26.23	0	68.81	66.7	26.23	25.4
		12*A10+4*A12+A38					[118]
$C_{17}H_{13}F_3O$		4-*n*-propoxy-2′,3′,4′-trifluorodiphenylacetylene					
	327.3	26.1	0	79.74	80.5	26.1	26.4
		6*A10+6*A12+3*A24+2*A2+A1+2*A9+A32					[196]
$C_{17}H_{14}F_2$		4-*n*-propyl-3′,4′-difluorodiphenylacetylene					
	311	20.2	0	64.95	72.0	20.2	22.4
		7*A10+A11+4*A12+2*A24+2*A2+A1+2*A9					[196]
$C_{17}H_{14}F_2O$		4-*n*-propoxy-2′,4′-difluorodiphenylacetylene					
	326.9	25.2	0	77.09	78.8	25.2	25.8
		7*A10+5*A12+2*A24+2*A2+A1+2*A9+A32					[196]
$C_{17}H_{14}N_2O_2$		2,2-bis-(4-cyanatophenyl)propane					
	355.8	26.69	0	75.02	71.7	26.69	25.51
		2*A1+A4+2*A11+2*A12+2*A58+8*A10					[216]
$C_{17}H_{14}O_5$		3-[1-(2-furanyl)-3-oxobutyl]-4-hydroxy-2H-1-benzopyran-2-one					
	391.8	33.88	0	86.49	87.5	33.88	34.3
		2*A14+5*A15+5*A19+2*A18+A18*B18+4*A10+A1					[221]
		+A2+A3+A35+A115+A112+A30*D30					
$C_{17}H_{15}F$		4-*n*-propyl-4′-fluorodiphenylacetylene					
	324	24.1	0	74.38	70.2	24.1	22.8
		8*A10+A11+3*A12+A24+2*A2+A1+2*A9					[196]
$C_{17}H_{15}FO$		4-*n*-propoxy-4′-fluorodiphenylacetylene					
	356.8	27.1	0	75.95	77.0	27.1	27.5
		8*A10+4*A12+A24+2*A2+A1+2*A9+A32					[196]
$C_{17}H_{16}Br_2O_3$		isopropyl 4,4′-dibromobenzilate					
	348.1	24.55	0	70.53	93.5	24.55	32.5
		8*A10+2*A11+2*A12+A30*D30+A38+2*A1+A3*B3+2*A21+A4*B4					[216]
$C_{17}H_{18}FN_3O_3$		1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-qiunolinecarboxylic acid					
	541.5	64.48	0	119.08	91.2	64.48	49.4
		3*A14+6*A15+3*A19+A18*B18+A114+2*A119					[36]
		+A121+2*A10+2*A12+A36*F36+A24					
$C_{17}H_{19}FNO_2$		4-*trans*-(3-fluoro-4-cyanophenyl)cyclohexyl (E)-but-2-enoate					
	393.2	21.1	0	53.66	81.5	21.1	32.0
		3*A10+2*A12+A11+A24+A56+A14+3*A15+2*A16+A38+A6+A6*B6+A1					[140]
$C_{17}H_{19}F_3O_3$		4-*trans*-(trifluoromethoxyphenyl)cyclohexyl (E)-but-2-enoate					
	340.2	21.6	0	63.49	83.6	21.6	28.4
		4*A10+A12+A11+3*A25+A14+3*A15+2*A16					[140]
		+A38+A6+A6*B6+A1+A32+A4*B4					
$C_{17}H_{21}NO_2$		N,N-diethyl-2-(1-naphthyloxy)propionamide					
	345.3	24.57	0	71.16	80.3	24.57	27.7
		3*A1+2*A2+B3*A3+7*A10+3*A12+A32+A59					[221]
$C_{17}H_{34}O$		9-heptadecanone					
	323.9	66.68	0	205.87	170.4	66.68	55.2
		2*A1+A35+A14*A2*B2					[21]
$C_{17}H_{34}O_2$		heptadecanoic acid					
	329.2	7.44	22.59				
	334.3	51.33	153.55	176.15	170.9	58.77	57.1
		15*A2*B2+A1+A36					[216]
$C_{17}H_{34}O_2$		methyl palmitate					
	307.2	68.16	0	221.84	173.5	68.16	53.3
	305.2	55.35		181.4		55.35	

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)	
		2*A1+14*A2*B2+A38					[217, 391]	C
$C_{17}H_{35}NO_3$		N-tetradecyl-L-alanine						
	367.1	52.3	0	142.47	157.6	52.3	57.9 [249]	C
		2*A1+13*A2*B2+A3*B3+A44+A36*B36						
$C_{17}H_{35}NO_3$		N-dodecyl-L-valine						
	380.1	33.1	0	87.08	140.2	33.1	53.3 [249]	C
		3*A1+A3+A3*B3+11*A2*B2+A44+A36*B26						
$C_{17}H_{35}NO_3$		N-dodecyl-DL-valine						
	364.6	64.4	0	176.63	140.2	64.4	51.1 [249]	C
		3*A1+A3+A3*B3+11*A2*B2+A44+A36*B36						
$C_{17}H_{36}$		*n*-heptadecane						
	284.3	10.96	38.56					
	295.1	40.17	136.11	174.67	175.1	51.13	51.7 [216]	C
		2*A1+15*A2*B2						
$C_{17}H_{36}O_2S$		3(*n*-tetradecylthio)-1,2-propanediol						
	302.5	16.3	53.88					
	336.4	26.8	79.67	133.55	179.6	43.1	60.4 [217]	C
		A1+13*A2*B2+A84+2*A30*C30+2*A2+A3*B3						
$C_{17}H_{36}O_3$		3(*n*-tetradecyloxy)-1,2-propanediol						
	331.3	62.1	0	187.44	182.2	62.1	60.4 [217]	C
		A1+13*A2*B2+A32+2*A30*C30+2*A2+A3*B3						
$C_{17}H_{37}NO_2$		3(*n*-tetradecylamino)-1,2-propanediol						
	356.2	64.9	0	182.2	172.2	64.9	61.3 [217]	C
		A1+13*A2*B2+A32+2*A30*C30+2*A2+A3*B3						
$C_{18}H_{10}$		benzofluoranthene						
	402.8	5.35	13.28					
	402.1	0.88	2.19					C
	352.7	0.44	1.23					
	424	11.8	27.83	44.53	36.1	18.47	15.3 [264]	C
		10*A10+5*A12+3*A13						
$C_{18}H_{12}$		triphenylene						
	471	24.74	0	52.53	44.1	24.74	20.8 [216]	C
		12*A10+6*A12						
$C_{18}H_{12}$		chrysene						
	512.2	3.22	6.29					
	531.4	26.15	49.21	55.5	44.1	29.37	23.4 [255]	C
		12*A10+6*A12						
$C_{18}H_{12}$		1,2-benzanthracene						
	434.3	21.38	0	49.23	44.1	21.38	19.1 [215]	C
		12*A10+6*A12						
$C_{18}H_{12}$		3,4-benzophenanthrene						
	334.7	16.32	0	48.75	44.1	16.32	14.8 [215]	C
		12*A10+6*A12						
$C_{18}H_{13}FO$		4-ethoxy-4′-fluorodiphenyldiacetylene						
	400.2	33.9	0	84.71	64.4	33.9	25.8 [195]	C
		A1+A2+4*A12+8*A10+4*A9+A24*B24+A32						
$C_{18}H_{14}$		*m*-terphenyl						
	360	22.59	0	62.76	73.9	22.59	26.6 [256]	C
		14*A10+4*A12						
$C_{18}H_{14}$		*p*-terphenyl						
	193.6	0.3	1.6					
	487	35.3	72.5	74.1	73.9	35.6	35.9 [38,155]	C
		14*A10+4*A12						
$C_{18}H_{14}$		*o*-terphenyl						
	329.4	17.2	0	52.3	73.9	17.2	24.3 [91]	C
		14*10+4*A12						
$C_{18}H_{14}O_3$		cinnamic anhydride						
	321.2	32.77	0	102.02	87.6	32.77	28.1 [215]	C
		10*A10+2*A12+A39+2*A6+2*A6*B6						
$C_{18}H_{15}F_3O$		4-*n*-butoxy-1′,3′,4′-trifluorodiphenylacetylene						
	344.4	36	0	104.53	87.7	36	30.2 [196]	C
		6*A10+6*A12+3*A24+A32+3*A2+A1+2*A9						
$C_{18}H_{15}ClSi$		triphenylchlorosilane						
	370.6	26.88	0	72.53	77.9	26.88	28.9 [216]	C
		15*A10+3*A12+A109+A22*B22						
$C_{18}H_{15}N$		triphenylamine						
	400.2	24.89	0	62.21	66.5	24.89	26.6 [217]	
		15*A10+3*A12+A43						

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{18}H_{15}OP$		triphenylphosphine oxide					
	431.9	24.22	0	56.08	56.1	24.22	24.2 [246]
		15*A10+3*A12+A73					
$C_{18}H_{15}O_4P$		triphenyl phosphate					
	322.5	29.61	0	91.81	78.8	29.61	25.4 [215]
		15*A10+3*A12+A74					
$C_{18}H_{15}P$		triphenylphosphine					
	354.4	19.69	0	55.56	68.0	19.69	24.1 [246]
		15*A10+3*A12+A72					
$C_{18}H_{16}F_2$		4-*n*-butyl-3′,4′-difluorodiphenylacetylene					
	323.5	25.3	0	78.21	79.1	25.3	25.6 [196]
		7*A10+A11+4*A12+2*A24+3*A2+A1+2*A9					
$C_{18}H_{16}O_3$		1,8-diphenyl-2,3,5-trioxabicyclo[4.3.0]non-7-ene					
	371.2	21.7	0	58.46	45.3	21.7	16.8 [257]
		10*A10+A11+A12+2*A14+3*A15+A19+A18+6*A16 +A17+A112+A113					
$C_{18}H_{16}O_8$		1,2,3,4-tetracarbomethoxynaphthalene					
	423.7	35.9	0	84.47	85.8	35.9	36.3 [217]
		4*A1+4*A38+4*A10+6*A12					
$C_{18}H_{16}O_8$		1,2,4,5-tetracarbomethoxynaphthalene					
	438.2	36.4	0	82.89	85.8	36.4	37.6 [217]
		4*A1+4*A38+4*A10+6*A12					
$C_{18}H_{16}O_8$		1,2,5,6-tetracarbomethoxynaphthalene					
	470.2	42.1	0	89.37	85.8	42.1	40.3 [217]
		4*A1+4*A38+4*A10+6*A12					
$C_{18}H_{16}O_8$		1,2,6,7-tetracarbomethoxynaphthalene					
	407.2	34.2	0	83.76	85.8	34.2	34.9 [217]
		4*A1+4*A38+4*A10+6*A12					
$C_{18}H_{16}O_8$		2,3,6,7-tetracarbomethoxynaphthalene					
	458.2	42.2	0	91.88	85.8	42.2	39.3 [217]
		4*A1+4*A38+4*A10+6*A12					
$C_{18}H_{16}O_8$		1,4,5,8-tetracarbomethoxynaphthalene					
	477.2	36.1	0	75.69	85.8	36.1	40.9 [217]
		4*A1+4*A38+4*A10+6*A12					
$C_{18}H_{17}Cl_2NO_3$		ethyl N-benzoyl-*n*-(3,4-dichlorophenyl)-*dl*-alaninate					
	341.7	27.06	0	79.19	90.9	27.06	31.1 [221]
		8*A10+4*A12+2*A1+A2+A3*B3+A38+2*A22*D22+A59					
$C_{18}H_{17}F$		4-*n*-butyl-4′-fluorodiphenylacetylene					
	329.9	18.5	0	56.08	77.4	18.5	25.5 [196]
		8*A10+A11+3*A12+A24+3*A2+A1+2*A9					
$C_{18}H_{17}FO$		4-*n*-butoxy-4′-fluorodiphenylacetylene					
	346.7	25.4	0	73.26	84.2	25.4	29.4 [196]
		8*A10+4*A12+A24+3*A2+A1+2*A9+A32					
$C_{18}H_{18}$		1-methyl-7-isopropylphenanthrene					
	369	18.03	0	48.87	46.6	18.03	17.2 [216]
		8*A10+3*A1+2*A11+A3+4*A12					
$C_{18}H_{18}ClNS$		2-chloro-9-(3-dimethylaminopropylidene)-10-thioxanthene					
	370.3	27.82	0	75.13	77.8	27.82	28.8 [216]
		A14+3*A15+2*A19+38*A19+A131+7*A10+A12+A22*C22+A6*B6 +2*A2+2*A1+A43					
$C_{18}H_{18}N_2O_2$		N,N′-(2-hydroxyethyl)-1,4-diaminoanthraquinone					
	521.2	32.34	0	62.05	86.0	32.34	44.8 [13]
		A14+3*A15+2*A114+4*A19+6*A10+2*A44+2*A12+4*A2+2*A30*D30					
$C_{18}H_{18}O_2$		3-diphenylmethyl-2,4-pentanedione					
	387.2	27.02	0	69.78	73.3	27.02	28.4 [259]
		2*A1+A3*B3+2*A35+A3+10*A10+2*A11					
$C_{18}H_{18}O_3$		butyl 9-hydroxy-9H-fluorene-9-carboxylate					
	343.9	25.56	0	74.31	81.2	25.56	27.9 [215]
		A14+2*A15+8*A10+4*A19+A17+A30*B30+A38+A1+3*A2					
$C_{18}H_{20}Cl_2$		1,1′-(2,2-dichloroethylidene)bis(4-ethylbenzene)					
	331.6	23.34	0	70.38	76.7	23.34	25.4 [215]
		8*A10+4*A11+A3+A3*B3+2*A1+2*A2+2*A22*B22					
$C_{18}H_{20}O_2$		diethylstilbestrol					
	443.8	31.76	0	71.57	97.8	31.76	43.5
	441.8	28.8	0	65.1	97.8	28.8	43.5 [221, 394]
		8*A10+4*A12+2*A31+2*A7+2*1+2*A2					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)	
$C_{18}H_{22}$		2,3-dimethyl-2,3-diphenylbutane						C_1
	392	25.52	0	65.11	55.6	25.52	21.8	
		10*A10+4*A1+2*A11+2*A4					[289]	
$C_{18}H_{22}N_4$		2,3-dimethyl-2,3-bis(phenylazo)butane						C_1
	342.3	21.09	0	61.6	76.8	21.09	26.3	
		4*A1+2*A4*B4+10*A10+2*A12+4*A42					[258]	
$C_{18}H_{22}O_2$		(*dl*) anisylidenecamphor						C_1
	371.5	26.36	0	70.95	67.9	26.36	25.2	
		2*A14+A15+4*A1+A114+A17+A16+A6+4*A10+2*A12+A32+A19+A17					[273]	
$C_{18}H_{22}O_2$		(*d*) anisylidenecamphor						C_1
	399.5	30.12	0	75.41	67.9	30.12	27.1	
		2*A14+A15+4*A1+A114+A17+A16+A6+4*A10+2*A12+A32+A19+A17					[273]	
$C_{18}H_{22}O_2$		di-α-cumyl peroxide						C_1
	312.4	28.14	0	90.08	90.1	28.14	28.2	
		4*A1+2*A4*B4+2*A11+10*A10+A33					[216]	
$C_{18}H_{23}FO_2$		4-*trans*-(4-fluorophenylethyl)cyclohexyl (E)-butenoate						C_1
	335.2	25	0	74.58	92.9	25	31.1	
		4*A10+A11+A12+2*A2+A14+3*A15+A16+A16+A38+A24+A1+A6+A6*B6					[140]	
$C_{18}H_{28}Si_4O_4$		1,1,3,3,5,5-hexamethyl-7,7-diphenylcyclotetrasiloxane						C_1
	305.0	42.73	0	140.12	78.4	42.73	23.9	
		6*A1+10*A10+2*A11+4*A112+4*A139+A14+5*A15					[216]	
$C_{18}H_{30}O$		2,4,6-tri-*tert*-butylphenol						C_1
	405.2	19.46	0	48.01	52.5	19.46	21.3	
		3*A11+2*A10+9*A1+3*A4+A31+A12					[220]	
$C_{18}H_{30}O_4$		*p*-diacetylbenzene diethyl ketal						C_1
	168.2	1.31	7.76					
	326.2	23.5	72.05	79.8	117.6	24.81	38.4	
		4*A10+2*A11+2*A4*B4+6*A1+4*A2+4*A32					[216]	
$C_{18}H_{32}O_2$		1,10-cyclooctadecanedione						C_1
	359.2	11.84	32.96					
	371.2	27.03	72.81	105.78	86.2	38.87	32.0	
		A14+15*A15+2*A114					[114]	
$C_{18}H_{32}O_4$		1,8-cyclotetradecanedione bis ethylene ketal						C_1
	457.2	30.67	0	67.08	84	30.67	38.4	
		3*A14+13*A15+2*A17+4*A112					[114]	
$C_{18}H_{34}O_2$		*trans*-9-octadecenoic acid (elaidic acid)						C_1
	317.6	61.55	0	193.8	172.1	61.55	54.7	
		A1+14*A2*B2+2*A6+A36					[216]	
$C_{18}H_{34}O_2$		*cis*-9-octadecenoic acid						C_1
	286.5	39.6	0	138.24	172.1	39.6	49.3	
		A1+14*A2*B2+2*A6+A36					[216]	
$C_{18}H_{34}O_2$		*cis*-6-octadecenoic acid						C_1
	303.7	47.5	0	156.43	172.1	47.5	52.3	
		A1+14*A2*B2+2*A6+A36					[216]	
$C_{18}H_{36}$		*n*-dodecylcyclohexane						C_1
	258.8	45.84	0	177.11	150.0	45.84	38.8	
		A14+A16+A1+11*A2*B2+3*A15					[216]	
$C_{18}H_{36}$		cyclooctadecane						C_1
	298.2	29.29	98.22					
	346.2	9.87	28.52	126.74	88.9	39.16	30.8	
		15*A15+A14					[110]	
$C_{18}H_{36}$		1,1-dimethylcyclohexadecane						C_1
	216.2	1.26	5.81					
	221.2	0.42	1.89					
	290.2	14.23	49.02	56.72	82.1	15.9	23.8	
		A14+13*A15+2*A1+A17					[112]	
$C_{18}H_{36}N_2O_2^*$		N,N′-di-*n*-hexyladipamide						C_1
	432	40.79	0	94.56	168.7	40.79	72.9	
		14*A2*B2+2*A1+2*A60					[216]	
$C_{18}H_{36}O_2$		octadecanoic acid						C_1
	342.5	61.21	0	178.66	180.2	61.21	61.7	
		16*A2*B2+A1+A36					[216]	
$C_{18}H_{36}O_2$		ethyl hexadecanoate						C_1
	296.4	15.09	0	50.93	180.6	15.09	53.5	
		2*A1+A38+14*A2*B2+A2					[216]	

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{18}H_{36}O_4$	2,2,11,11-tetramethyl-1,3,10,12-tetraoxacyclooctadecane					
373.0	35.1	0	94.1	94.9	35.1	35.4
	$A14+15*A15+4*A112+2*A17+4*A1$					[47]
$C_{18}H_{37}NO$	N-butyl tetradecanamide					
336.1	45	0	133.89	170.0	45	57.1
	$2*A1+3*A2+A60+12*A2*B2$					[217]
$C_{18}H_{37}NO$	octadecanamide					
377.2	59.91	0	158.84	194.8	59.91	73.5
	$16*A2*B2+A1+A61$					[217]
$C_{18}H_{37}NO_3$	N-hexadecylglycine					
384.6	4.5	11.7				
366.1	5.6	15.3				
393.1	56.5	143.73	170.73	175.5	66.6	69.0
	$15*A2*B2+A1+A44+A36*B36+A2$					[249]
$C_{18}H_{37}NO_3$	N-dodecyl-L-luecine					
383.1	33.5	0	87.44	147.3	33.5	56.4
	$3*A1+11*A2*B2+A3+A3*+A36*B36+A44+A2$					[249]
$C_{18}H_{37}NO_3$	N-dodecyl-DL-leucine					
341.1	28.9	84.73				
356.6	31	86.93	171.66	147.3	59.9	52.5
	$3*A1+11*A2*B2+A3+A3*B3+A36*B36+A44+A2$					[249]
$C_{18}H_{38}$	octadecane					
301.3	61.5	0	204.6	184.5	61.5	55.6
	$2*A1+16*A2*B2$					[216]
$C_{18}H_{38}O$	octadecanol					
334.2	70.08	0	209.7	178.0	70.08	59.5
	$17*A2*B2+A1+A30$					[220]
$C_{18}H_{48}Si_6$	1,2,3,4,5,6-hexamethyl-1,2,3,4,5,6-hexaethylcyclohexasilane					
226.3	3.8	16.79				
439.2	1.8	4.1	20.89	90.1	5.6	39.6
	$A14+3*A15+6*A139+12*A1+6*A2$					[175]
$C_{19}H_{13}F_3O$	4-ethoxy-4′-trifluoromethyldiphenyldiacetylene					
424.9	32.73	0	77.03	62.9	32.73	26.7
	$A1+A2+A11+3*A12+8*A10+4*A9+3*A25+A4*B4+A32$				-	[195]
$C_{19}H_{14}F_2$	4-*n*-propyl-3′,4′difluorodiphenyldiacetylene					
343.7	22.03	0	64.1	66.4	22.03	22.8
	$A1+2*A2+A11+4*A12+7*A10+4*A9+2*A24$					[195]
$C_{19}H_{15}Cl$	triphenylchloromethane					
376.8	27.9	0	74.04	70.3	27.9	26.5
	$15*A10+3*A11+A22+A4*B4$					[216]
$C_{19}H_{16}$	triphenylmethane					
365.3	21.97	0	60.13	66.0	21.97	24.1
	$15*A10+A3+3*A11$					[216]
$C_{19}H_{16}O_2$	2-fluorenyl-2-methyl-1,3-cyclopentanedione					
395.2	24.6	0	62.25	57.4	24.6	22.7
	$2*A14+4*A15+2*A114+A17+A1+A16+4*A19+8*A10$					[259]
$C_{19}H_{17}F_3O$	4-*n*-pentoxy-2′,3′,4′-trifluorodiphenylacetylene					
315.8	33.1	0	104.81	94.8	33.1	29.9
	$6*A10+6*A12+3*A24+A32+4*A2+A1+2*A9$					[196]
$C_{19}H_{18}F_2$	4-*n*-pentyl-3′,4′-difluorodiphenylacetylene					
323.1	22.1	0	68.4	86.2	22.1	27.9
	$7*A10+A11+4*A12+2*A24+4*A2+A1+2*A9$					[196]
$C_{19}H_{18}O_2$	2-methyl-2-diphenylmethyl-1,3-cyclopentanedione					
394.2	34.3	0	87.01	59.7	34.3	23.5
	$A14+2*A15+2*A114+A17+A1+A3+2*A11+10*A10$					[259]
$C_{19}H_{19}F$	4-*n*-pentyl-4′-fluorodiphenylacetylene					
337.4	25.6	0	75.87	84.5	25.6	28.5
	$8*A10+A11+3*A12+A24+4*A2+A1+2*A9$					[196]
$C_{19}H_{19}FO$	4-*n*-pentoxy-4′-fluorodiphenylacetylene					
330.9	27.2	0	82.2	91.3	27.2	30.2
	$8*A10+4*A12+A24+4*A2+A1+2*A9+A32$					[196]
$C_{19}H_{20}F_3N_3O_3$	2-[3-(trifluoromethyl)-phenyl]amino-3-pyridinecarboxylic acid β-morpholino ethyl ester					
350	34.5	0	98.57	91.1	34.5	31.9
	$A14+3*A15+A112+A119+2*A2+A38+7*A10+3*A12+A41+A44+A11+A4*B4+3*A25$					[216]
$C_{19}H_{20}O_2$	3-methyl-3-diphenylmethyl-2,4-pentanedione					
352.2	25.1	0	71.27	77.6	25.1	27.3

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
							[259]
		$3*A1+A4*B4+2*A35+A3+10*A10+2*A11$					
$C_{19}H_{21}NO$		1,2-diphenyl-2-(N-piperidinyl)-1-ethanone					
	349.2	33.93	0	97.16	77.0	33.93	26.9
		$10*A10+A11+A12+A35+A14+3*A15+A119+A3*B3$					[253]
$C_{19}H_{23}NO$		*p-n*-hexyloxybenzylideneaniline					
	73.41	0.19	2.62				
	321.6	30.91	96.1	98.72	104.4	31.1	33.58
		$9*A10+3*A12+A42+A32+5*A2+A1+A6*B6$					[216]
$C_{19}H_{24}O$		2-*tert*-butyl-4-methyl-6-α-methylbenzylphenol					
	337.7	31.38	0	92.92	63.0	31.4	21.3
		$5*A1+A4+4*A11+A12+7*A10+A31+A3$					[101]
$C_{19}H_{26}O_2$		testosterone					
	428	29.45	0	68.81	60.2	29.45	25.9
		$4*A14+5*A15+2*A17+4*A16+2*A1+A30*B30+A19+A18*B18+A114$					[219]
$C_{19}H_{28}N_2$		4-(4-*n*-heptyl-1-piperidinyl)benzonitrile					
	326.2	29.01	0	88.95	103.2	29.1	33.7
		$A14+3*A15+A119+A16+6*A2+A1+4*A10+2*A12+A56$					[26]
$C_{19}H_{30}O_2$		5α-androstane-3-one-17β-ol					
	455.5	27.15	0	59.6	60.9	27.15	27.7
		$4*A14+5*A15+2*A17+2*A1+5*A16+A30*B30+A114$					[216]
$C_{19}H_{38}O$		2-nonadecanone					
	328	68.65	0	209.3	189.0	68.65	62.0
		$A35+2*A1+16*A2*B2$					[21]
$C_{19}H_{38}O$		10-nonadecanone					
	330	66.67	0	202.04	189.0	66.67	62.4
		$A35+2*A1+16*A2*B2$					[21]
$C_{19}H_{38}O_2$		nonadecanoic acid					
	338	9.76	28.87				
	341.2	57.62	168.87	195.93	189.6	67.38	64.7
		$17*A2*B2+A1+A36$					[216]
$C_{19}H_{38}O_2$		methyl octadecanoate					
	310.9	64.4	0	205.8	192.1	64.4	59.7
		$2*A1+A38+16*A2*B2$					[391]
$C_{19}H_{39}NO_3$		N-hexadecyl-L-alanine					
	374.1	65.3	0	174.55	176.3	65.3	66.0
		$15*A2*B2+2*A1+A3*B3+A44+A36*B36$					[249]
$C_{19}H_{39}NO_3$		N-tetradecyl-L-valine					
	334.6	14.9	44.53				
	365.1	20.6	56.42	100.95	158.8	35.5	58.0
		$3*A1+A3+A3*B3+13*A2*B2+A44+A36*B36$					[249]
$C_{19}H_{39}NO_3$		N-tetradecyl-DL-valine					
	370.1	68.1	0	184	158.8	68.1	58.8
		$3*A1+A3+A3*B3+13*A2*B2+A44+A36*B36$					[249]
$C_{19}H_{40}$		nonadecane					
	296.0	13.67	46.2				
	304	47.4	155.9	202.1	193.8	61.07	58.7
		$2*A1+17*A2*B2$					[216]
$C_{20}F_{42}$		perfluoroeicosane					
	149.5	0.67	4.48				
	202.9	11.25	55.45				
	437.9	80.33	183.44	243.37	211.6	92.25	92.6
		$20*A4*B4+36*A26+6*A25$					[67]
$C_{20}H_{12}$		perylene					
	551.0	31.88	0	57.87	43.7	31.88	24.1
		$12*A10+6*A12+2*A13$					[216, 217]
$C_{20}H_{12}$		1,2-benzopyrene					
	426.2	2.51	5.89				
	454.4	16.57	36.46	42.35	43.7	19.08	19.8
		$12*A10+6*A12+2*A13$					[215]
$C_{20}H_{12}$		3,4-benzopyrene					
	390.2	8.49	21.77				
	454.2	17.32	38.13	59.9	43.7	25.81	19.8
		$12*A10+6*A12+2*A13$					[215]
$C_{20}H_{14}$		triptycene					
	527.2	30.29	0	57.46	60.1	30.29	31.7
		$2*A14+2*A15+2*A16+6*A19+12*A10$					[216]
$C_{20}H_{14}$		β,β-binaphthyl					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
	461.2	38.9	0	84.35	58.9	38.9	27.2
		14*A10+6*A12					[216]
$C_{20}H_{14}O_4$		phenolphthalein					
	534	51.05	0	95.59	114.34	51.05	61.06
		A14+2*A15+A115+2*A19+A17+2*A31+12*A10					[216]
$C_{20}H_{15}F_3O$		4-propoxy-4′-trifluoromethyldiphenyldiacetylene					
	315.9	18.81	0	59.54	70.0	18.81	22.1
		A1+2*A2+A11+3*A12+8*A10+4*A9+3*A25+A4*B4+A32					[195]
$C_{20}H_{16}F_2$		4-*n*-butyl-3′,4′-diflurodiphenyldiacetylene					
	340.8	24.33	0	71.39	73.6	24.33	25.1
		A1+3*A2+A11+4*A12+7*A10+4*A9+2*A24					[195]
$C_{20}H_{18}O_2$		2-fluoroenyl-2-methyl-1,3-cyclohexanedione					
	448.2	35.7	0	79.65	61.1	35.7	27.4
		2*A14+5*A15+2*A114+A17+A1+A16+4*A19+8*A10					[259]
$C_{20}H_{18}O_2Sn$		(acetyloxy)triphenylstannane					
	397.6	41.92	0	105.44	89.8	41.92	35.7
		15*A10+3*A12+A1+A38+A110					[221]
$C_{20}H_{19}F_3O$		4-*n*-hexyloxy-2′,3′,4′-trifluorodiphenylacetylene					
	322	30.8	0	95.65	85.3	30.8	27.5
		A1+5*A2+6*A12+6*A10+2*A9+2*A24+A32					[196]
$C_{20}H_{20}F_2$		4-*n*-hexyl-3′,4′-difluorodiphenylacetylene					
	314.9	24.3	0	77.17	78.5	24.3	24.7
		A1+5*A2+A11+5*A12+6*A10+2*A9+2*A24					[196]
$C_{20}H_{20}F_2O$		4-*n*-hexyloxy-3′,4′-difluorodiphenylacetylene					
	323.6	33.1	0	102.29	85.3	33.1	27.6
		A1+5*A2+6*A12+6*A10+2*A9+2*A24+A32					[196]
$C_{20}H_{20}F_2O$		4-*n*-hexyloxy-2′,4′-difluorodiphenylacetylene					
	320.9	34.1	0	106.26	85.3	34.1	27.4
		A1+5*A2+6*A12+6*A10+2*A9+2*A24+A32					[196]
$C_{20}H_{20}O_2$		2-ethyl-2-diphenylmethyl-1,3-cyclopentanedione					
	382.2	28.2	0	73.78	66.8	28.2	25.5
		A14+2*A15+2*A114+A17+A1+A3+2*A11+10*A10+A2					[259]
$C_{20}H_{20}O_3$		4,4-dimethyl-1,8-diphenyl-2,3,5-trioxabicyclo[4.3.0]non-7-ene					
	369.2	22.1	0	59.86	45.9	22.1	16.9
		10*A10+A11+A12+2*A14+3*A15+A19+A18+A162+A17+A112+A113+2*A1					[257]
$C_{20}H_{22}O_2$		3-ethyl-3-diphenylmethyl-2,4-pentanedione					
	388.2	34.7	0	89.39	84.8	34.7	32.9
		3*A1+A4*B4+2*A35+A3+10*A10+2*A11+A2					[259]
$C_{20}H_{26}O_2$		19-nor-17α-ethylnyltestosterone					
	479	39.6	0	82.67	55.1	39.6	26.4
		4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114					[216]
		+A30*B30+A1+A8+A9					
$C_{20}H_{26}O_2$		2-*tert*-butyl-4-methoxymethyl-6-α-methylbenzylphenol					
	371.7	29.4	0	79.1	74.8	29.4	27.8
		5*A1+A4+A2+A3+4*A11+A12+7*A10+A31+A32					[101]
$C_{20}H_{26}O_3$		testosterone formate					
	398	26.36	0	66.22	66.2	26.36	26.4
	398.2	18.12	0	45.5	66.2	18.1	26.4
		4*A14+5*A15+2*A17+4*A16+2*A1+A37+A19+A18*B18+A114					[219, 396]
$C_{20}H_{28}O_2$		1-[3,5-di-*tert*-butyl-4-hydroxyphenyl]-5-hexyn-1-one					
	342.2	25.14	0	73.47	74.9	25.14	25.6
		6*A1+2*A4+2*A10+2*A11+2*A12+3*A2+A8+A9+A31+A35					[39]
$C_{20}H_{30}O_3Si_3$		1,1,3,3-tetraethyl-5,5-diphenylcyclotrisiloxane					
	279.1	18.37	0	65.84	97.9	18.37	27.3
		4*A1+4*A2+10*A10+2*A11+3*A112+3*A139+A14+3*A15					[216]
$C_{20}H_{32}$		10,10,13,13-tetramethylcyclohexadeca-1,5-diyne					
	323.2	18.83	0	58.25	63.8	18.83	20.6
		4*A1+A14+13*A15+2*A17+4*A20					[113]
$C_{20}H_{36}O_2$		1,10-cycloeicosanedione					
	327.2	55.06	0	168.28	98.7	55.06	32.3
		A14+17*A15+2*A112					[114]
$C_{20}H_{36}O_4$		1,9-cyclohexadecanedione bis ethylene ketal					
	404.2	42.13	0	104.24	91.4	42.13	36.9
		3*A14+15*A15+2*A17+4*A112					[114]
$C_{20}H_{40}$		1,1,9,9-tetramethylcyclohexadecane					
	364.2	25.1	0	68.93	82.6	25.1	30.1
		4*A1+A14+13*A15+2*A17					[112]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{20}H_{40}$	303.2	1,1,4,4-tetramethylcyclohexadecane 25.1 4*A1+A14+13*A15+2*A17	0	82.8	82.6	25.1	25.1 [112]
$C_{20}H_{40}$	283.2	1,1-dimethylcyclooctadecane 23.85 A14+15*A15+2*A1+A17	0	84.21	89.5	23.85	25.3 [110]
$C_{20}H_{40}O_2$	348.2	eicosanoic acid 69.2 18*A2*B2+A1+A36	0	198.7	198.9	69.2	69.3 [216]
$C_{20}H_{40}O_4$	406.9	2,2,6,6,10,10,14,14-octamethyl-1,3,9,11-tetraoxacyclohexadecane 24.69 8*A1+2*A17+2*A17+A14+13*A15+4*A112	0	60.67	88.7	24.69	36.1 [117]
$C_{20}H_{41}NO$	310 328 334	N-hexyl tetradecanamide 8 7 35 2*A1+17*A2*B2+A60	25.81 21.34 104.79	151.94	195.2	50	65.2 [260]
$C_{20}H_{41}NO_3$	377.5	N-tetradecyl-L-leucine 32.4 3*A1+13*A2*B2+A3+A3*B3+A2+A44+A36*B36	0	85.83	166.0	32.4	62.7 [249]
$C_{20}H_{41}NO_3$	320.1 349.6	N-tetradecyl-DL-leucine 1.8 54.8 3*A1+13*A2*B2+A3+A3*B3+A2+A44+A36*B36	5.62 156.75	162.37	166.0	56.6	58.0 [249]
$C_{20}H_{42}$	308.8	*n*-eicosane 67.8 2*A1+18*A2*B2	0	219.6	203.1	67.8	62.7 [216]
$C_{21}H_{16}$	369.6	1,2′-dinaphthylmethane 30.54 14*A10+2*A11+A2+4*A12	0	82.64	61.8	30.54	22.8 [216]
$C_{21}H_{17}F_3O$	414.3	4-*n*-butoxy-4′-trifluoromethyldiphenyldiacetylene 25.37 A1+3*A2+A11+3*A12+8*A10+4*A9+3*A25+A4*B4+A32	0	61.24	77.1	25.37	32.0 [195]
$C_{21}H_{18}F_2$	355.1	4-*n*-pentyl-3′,4′-difluorodiphenyldiacetylene 30.86 A1+4*A2+A11+4*A12+7*A10+4*A9+2*A24	0	86.91	80.7	30.86	28.7 [195]
$C_{21}H_{21}NO$	402	N,N-dimethyl-2,2-diphenylbenzeneacetamide 25.43 15*A10+3*A11+A4*B4+2*A1+A59	0	63.26	83.5	25.43	33.6 [221]
$C_{21}H_{24}O_2$	349.2	3-propyl-3-diphenylmethyl-2,4-pentanedione 27.1 3*A1+A4*B4+2*A35+A3+10*A10+2*A11+2*A2	0	77.61	91.9	27.1	32.1 [259]
$C_{21}H_{24}O_3Si_3$	374.3	*cis*-1,3,5-trimethyl-1,3,5-triphenylcyclotrisiloxane 43.07 3*A1+15*A10+3*A11+3*A112+3*A139+A14+3*A15	0	115.07	79.2	43.07	29.7 [216,99]
$C_{21}H_{24}O_3Si_3$	320.9	*trans*-1,3,5-trimethyl-1,3,5-triphenylcyclotrisiloxane 43.66 3*A1+15*A10+3*A11+3*A112+3*A139+A14+3*A15	0	136.07	79.2	43.66	25.4 [216,99]
$C_{21}H_{28}O_3$	413 413.2	testosterone acetate 27.88 22.5 4*A14+5*A15+2*A17+4*A16+3*A1+A19+A18*B18+A114+A38	0 0	67.51 54.5	67.7 67.7	27.88 22.5	27.9 27.9 [219, 396]
$C_{21}H_{28}O_5$	513	prednisolone 38.86 4*A14+5*A15+2*A17+A17+4*A16+2*A1 +3*A30*E30+A19+2*A18*B18+A18+A114+A35+A2	0	75.75	78.2	38.86	40.1 [219]
$C_{21}H_{28}O_5$	495	cortisone 36.86 4*A14+5*A15+A17+2*A17+3*A16+2*A1+2*A30*E30 +A19+A18*B18+2*A114+A35+A2	0	74.46	74.1	36.86	37.2 [219]
$C_{21}H_{30}O_2$	404	progesterone 26.99 4*A14+5*A15+2*A17+4*A16+3*A1+A19+A18*B18+A114+A35	0	66.8	64.6	26.99	26.1 [219]
$C_{21}H_{30}O_3$	414	deoxycorticosterone 27.98 4*A14+5*A15+2*A17+4*A16+2*A1+A30*C30 +A19+A18*B18+2*A114+A35+A2	0	67.59	69.4	27.98	28.9 [219]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{21}H_{30}O_4$		corticosterone					
	454	33.32	0	73.39	84.1	33.32	38.7
		4*A14+5*A15+2*A17+5*A16+2*A1+2*A30*D30+A19+A18*B18+A114+A35+A2					[219]
$C_{21}H_{30}O_5$		hydrocortisone					
	486	35.84	0	73.75	82.9	35.84	40.3
		4*A14+5*A15+3*A17+4*A16+2*A1+					[219]
		3*A30*E30+A19+A18*B18+A114+A35+A2					
$C_{21}H_{35}N_3N_2$		N-palmitoyl-pyrazinamide					
	362.7	51.82	0	142.87	192.5	51.82	69.8
		A1+14*A2*B2+3*A10+A12+2*A41+A71					[261]
$C_{21}H_{42}O$		11-heneicosanone					
	336.7	76.2	0	226.31	207.7	76.2	69.9
		2*A1+A35+18*A2*B2					[262]
$C_{21}H_{42}O$		2-heneicosanone					
	333.9	77.65	0	232.55	207.7	77.65	69.4
		2*A1+A35+18*A2*B2					[263]
$C_{21}H_{43}NO_3$		N-hexadecyl-L-valine					
	349.1	29.1	83.36				
	366.6	54.8	149.48	232.84	177.5	83.9	65.1
		3*A1+A3+A3*B3+15*A2*B2+A44+A36*B36					[249]
$C_{21}H_{43}NO_3$		N-hexadecyl-DL-valine					
	375.1	80.5	0	214.61	177.5	80.5	66.6
		3*A1+A3+A3*B3+15*A2*B2+A44+A36*B36					[249]
$C_{21}H_{44}$		*n*-heneicosane					
	305.7	15.48	50.65				
	313.7	47.7	152.06	202.71	212.4	63.18	66.6
		19*A2*B2+2*A1					[216]
$C_{22}H_{12}$		1,12-benzoperylene					
	554.2	17.37	0	31.34	43.2	17.37	24.0
		12*A10+4*A13+6*A12					[215]
$C_{22}H_{12}$		*o*-phenylenepyrene					
	435.2	21.51	0	49.41	36.0	21.51	15.7
		A14+2*A15+5*A19+12*A10+2*A13+3*A12					[264]
$C_{22}H_{14}$		picene					
	637.2	35.19	0	55.22	44.0	35.19	28.0
		14*A10+8*A12					[264]
$C_{22}H_{14}$		1,2:3,4-dibenzanthracene					
	553.5	25.82	0	46.65	44.0	25.82	24.3
		14*A10+8*A12					[215]
$C_{22}H_{14}$		1,2:5,6-dibenzanthracene					
	544.2	31.16	0	57.26	44.0	31.16	23.9
		14*A10+8*A12					[215]
$C_{22}H_{14}O_4$		1,4-bis(phenylglyoxaloyl)benzene					
	425.1	32.3	0	75.98	92.2	32.3	39.2
		14*A10+4*A12+4*A35					[216]
$C_{22}H_{18}F_2O$		4-(6-hexenyloxy)-3′,4′-difluorodiphenyldiacetylene					
	370	37.45	0	101.22	92.5	37.45	34.2
		A5+A6+4*A2+5*A12+7*A10+4*A9+2*A24+A32					[195]
$C_{22}H_{18}F_2O$		4-(*cis*-4-hexenyloxy)-3′,4′-difluorodiphenyldiacetylene					
	364.4	35.32	0	96.93	90.9	35.32	33.1
		A1+2*A6+3*A2+5*A12+7*A10+4*A9+2*A24+A32					[195]
$C_{22}H_{18}F_2O$		4-(*cis*-3-hexenyloxy)-3′,4′-difluorodiphenyldiacetylene					
	364.6	30.97	0	84.94	91.0	30.97	33.1
		A1+2*A6+3*A2+5*A12+7*A10+4*A9+2*A24+A32					[195]
$C_{22}H_{19}Br_2NO_3$		(S)-α-cyano-3-phenoxybenzyl (1R)-*cis*-3-(2,2-dibromovinyl)-2,2-dimethylcyclopropanecarboxylate					
	372.9	40.71	0	109.18	96.6	40.71	36.0
		A14+A17+2*A16+2*A1+A6+A7+2*A21					[221]
		+A38+A3*B3+A56+2*A12+A11+9*A10+A32					
$C_{22}H_{24}O_3$		4-methyl-4-propyl-1,8-diphenyl-2,3,5-trioxabicyclo[4.3.0]non-7-ene					
	351.2	16.6	0	47.27	60.1	16.6	21.1
		10*A10+A11+A12+2*A14+3*A15+A19+A18+A16+2*A17+A112+A113+2*A1+2*A2					[257]
$C_{22}H_{28}$		1,1′-diphenyl-1,1′-bicyclopentyl					
	414	31.38	0	75.77	67.4	31.38	27.9
		2*A14+4*A15+2*A17+2*A11+10*A10					[289]