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)
$C_5H_{10}O_2$		2,2-dimethylpropanoic acid (pivalic acid)					
	278.3	8.18	29.39				
	309.1	2.27	7.34	36.74	43.3	10.45	13.4
		$3*A1+A4*B4+A36$					[180]
$C_5H_{10}O_4$		2,2-bis-hydroxymethylpropanoic acid					
	426	38.5	90.37				
	468	3.59	7.68	98.05	73.0	42.09	34.2
		$A1+2*A2+A4*B4+A36*C36+2*A30*C30$					[216]
$C_5H_{10}O_5$		pentacycloformaldehyde					
	334	21.9	0	65.6	65.4	21.9	21.8
		$7*A15+A14+5*A112$					[216]
$C_5H_{10}S$		2-methylcyclothiapentane					
	172.4	8.87	0	51.48	46.5	8.87	8.0
		$A14+2*A15+A1+A16+A131$					[216]
$C_5H_{10}S$		3-methylcyclothiapentane					
	192	10.37	0	54	46.5	10.37	8.9
		$A14+2*A15+A1+A16+A131$					[216]
$C_5H_{10}S$		thiacyclohexane					
	201.4	1.1	5.44				
	240.0	7.77	32.38				
	292.3	2.45	8.37	46.19	47.4	11.32	13.9
		$A14+3*A15+A131$					[216]
$C_5H_{10}S$		cyclopentanethiol					
	155.4	7.83	0	50.38	49.1	7.83	7.6
		$A14+2*A15+A86+A16$					[288]
$C_5H_{11}Br$		1-bromopentane					
	185.1	14.37	77.61	77.61	72.5	14.37	13.4
		$4*A2*B2+A1+A21$					[216]
$C_5H_{11}N$		cyclopentylamine					
	184.5	0.48	2.58				
	190.4	8.31	43.65	46.23	47.4	8.79	9.0
		$A14+2*A15+A45+A16$					[216]
$C_5H_{11}NO$		piperidine					
	262.1	14.85	0	56.64	46.7	14.85	12.2
		$A14+3*A15+A121$					[216]
$C_5H_{11}NO_2$		N-methylmorpholine-N-oxide					
	457.4	18.8	0	41.1	41.1	18.8	18.8
		$A14+3*A15+A112+A122+A1$					[151]
$C_5H_{11}NO_2$		2-amino-2-methyl-1,3-propanediol					
	351.3	24.68	70.26				
	383.6	2.73	7.12	77.38	64.4	27.41	24.7
		$A1+2*A2+A4*B4+2*A30*C30+A45$					[216]
$C_5H_{11}NO_3S$		2-methyl-2-(methylsulfonyl)propanal oxime					
	382.0	27.12	0	71.01	47.6	27.12	18.2
		$3*A1+A4*B4+A6*B6+A88+A53$					[221]
C_5H_{12}		pentane					
	143.5	8.4	0	58.58	63.2	8.4	9.1
		$2*A1+3*A2*B2$					[215]
C_5H_{12}		2-methylbutane					
	113.4	5.13	0	45.23	43.5	5.13	4.9
		$3*A1+A3+A2$					[216]
C_5H_{12}		2,2-dimethylpropane					
	140	2.58	18.41				
	256.5	3.26	12.69	31.1	35.5	5.83	5.0
		$4*A1+A4$					[216]
$C_5H_{12}NO_3PS$		O,O-dimethyl S-[2-(methylamino)-2-oxoethyl] phosphorodithioate					
	321.0	20.49	0	63.85	51.7	20.49	16.6
		$3*A1+A60+A2+A80$					[221]
$C_5H_{12}N_2O$		N-butylurea					
	313.1	7.02	22.42				
	344.9	0.88	2.55				
	369.3	14.55	39.4	64.37	68.1	22.45	25.1
		$3*A2*B2+A1+A67$					[215]
$C_5H_{12}N_2O$		N-*tert*-butylurea					
	249	0.1	0.41				
	449.8	33.13	73.65	74.06	52.4	33.23	23.6
		$3*A1+A4*B4+A67$					[215]
$C_5H_{12}N_2O$		1,1-diethylurea					
	197.3	2.07	10.49				
	342.3	16.78	49.02	59.51	68.9	18.85	23.6
		$2*A1+2*A2+A65$					[215, 124, 138]

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)
$C_5H_{12}N_2O$		1,3-diethylurea					
	339.4	1.87	5.51				
	383.4	12.46	32.5	38.01	50.9	14.33	19.5
		2*A1+A66+2*A2					[215, 124, 138]
$C_5H_{12}N_2O$		tetramethylurea					
	272.2	13.4	0	49.23	51.0	13.4	13.9
		4*A1+A63					[216]
$C_5H_{12}N_2O_2$		N-methyl-N-nitrobutanamine					
	331	37.56	0	113.46	101.7	37.56	33.7
		2*A1+3*A2+A51+A47					[225]
$C_5H_{12}O$		2,2-dimethyl-1-propanol					
	146	1.96	13.43				
	213	0.17	0.79				
	264	4.46	16.88	31.1	26.8	6.59	7.1
		3*A1+A4+A2+A30					[277]
$C_5H_{12}O$		1-pentanol					
	195.6	10.5	0	53.7	56.7	10.5	11.1
		A1+4*A2*B2+A30					[216]
$C_5H_{12}O$		methyl *tert*-butyl ether					
	164.6	7.6	0	46.19	52.2	7.6	8.6
		4*A1+A4*B4+A32					[216]
$C_5H_{12}O$		ethyl propyl ether					
	145.7	8.39	0	57.61	61.3	8.39	8.9
		2*A1+3*A2+A32					[216]
$C_5H_{12}O$		methyl *n*-butyl ether					
	157.5	10.85	0	68.9	61.3	10.85	9.7
		2*A1+3*A2+A32					[216]
$C_5H_{12}O_2$		1,5-pentanediol					
	248	15.72	0	63.6	82.9	15.72	20.6
		5*A2*B2+2*A30*B30					[216]
$C_5H_{12}O_2$		2-methyl-2-butanol					
	146	1.96	13.44				
	213	0.17	0.78				
	264	4.46	16.88	31.1	38.8	6.59	10.2
		3*A1+A4*B4+A2+A30					[216]
$C_5H_{12}O_2$		2,2-dimethyl-1,3-propanediol					
	315.2	13.8	43.78				
	403.2	4.6	11.41	55.19	50.8	18.4	20.5
		2*A1+2*A2+A4+2*A30*B30					[90]
$C_5H_{12}O_3$		2-hydroxymethyl-2-methyl-1,3-propanediol					
	354	23.17	65.46				
	470	5.38	11.44	76.91	55.1	28.55	25.9
		A1+3*A2+A4+3*A30*C30					[216]
$C_5H_{12}O_4$		pentaerythritol					
	460.4	43.93	95.4				
	538.7	7.11	13.2	108.78	85.4	51.04	46.0
		A4+4*A2+4*A30*D30					[216]
$C_5H_{12}O_5$		1,2,3,4,5-pentahydroxypentane (Ribitol)					
	374.7	37.6	0	100.35	90.4	37.6	39.9
		2*A2+3*A3*B3+5*A30*E30					[216]
$C_5H_{12}O_5$		1,2,3,4,5-pentahydroxypentane (Xylitol)					
	365.7	37.4	0	102.27	90.4	37.4	33.1
		2*A2+3*A3*B3+5*A30*E30					[216]
$C_5H_{12}O_5$		1,2,3,4,5-pentahydroxypentane (D-Arabitol)					
	379.4	38.9	0	102.53	90.4	38.9	34.3
		2*A2+3*A3*B3+5*A30*E30					[216]
$C_5H_{12}S$		methyl *tert*-butyl sulfide					
	190.8	8.41	0	44.1	49.6	8.41	9.5
		4*A1+A4*B4+A84					[216]
$C_5H_{12}S$		ethyl propyl sulfide					
	156.1	10.58	0	67.8	58.7	10.58	9.2
		2*A1+3*A2+A84					[216]
$C_5H_{12}S$		methyl butyl sulfide					
	175.6	12.45	0	70.9	58.7	12.45	10.3
		2*A1+3*A2+A84					[136]
$C_5H_{12}S$		3-methyl-1-butanethiol					
	139.6	7.41	0	53.05	56.1	7.41	7.8
		2*A1+A3+2*A2+A86					[216]
$C_5H_{12}S$		1-pentanethiol					
	197.5	17.53	0	88.78	77.9	17.53	15.4

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)
		A1+4*A2*B2+A86					[216]
$C_5H_{12}S$		2-methyl-2-butanethiol					
	144.5	7.06	48.87				
	146.1	0.61	4.15	53.01	60.0	7.67	8.8
		3*A1+A4*B4+A2+A86					[105]
$C_5H_{12}S$		3-methyl-2-butanethiol					
	144.5	7.06	48.89				
	146.1	0.61	4.16	53.05	49.7	7.67	7.3
		3*A1+A3+A3*B3+A86					[216]
$C_5H_{12}SO_2$		*tert*-butylmethylsulfone					
	357.6	24.69	0	69.03	47.7	24.69	17.1
		4*A1+A4*B4+A88					[276]
$C_5H_{12}S_4$		tetra(methylthia)methane					
	296.4	6.11	20.5				
	318.7	7.61	23.85				
	338.7	4.14	12.13	56.48	55.9	14.78	18.9
		4*A1+A4*B4+4*A84					[216]
$C_5H_{12}Si$		1,1-dimethyl-1-silacyclobutane					
	155.5	6.76	42.87	43.48	37.6	6.76	5.8
		A14+A15+A139+2*A1					[153]
$C_5H_{12}Si$		vinyltrimethylsilane					
	141.7	7.66	0	54.06	46.9	7.66	6.6
		3*A1+A5+A6*B6+A109					[216]
$C_5H_{14}N_2$		N,N-dimethyl-1,3-propanediamine					
	194.4	12.38	0	63.7	55.7	12.38	10.8
		2*A1+3*A2+A43+A45					[216]
C_6ClF_5		chloropentafluorobenzene					
	191	3.64	19.04				
	245	0.98	4.01				
	257.5	8.36	32.45	55.5	54.5	12.36	14.0
		5*A24+A22*B22+6*A12					[216]
$C_6Cl_3F_3$		1,3,5-trichloro-2,4,6-trifluorobenzene					
	335.0	19.83	0	59.2	53.6	19.83	17.9
		3*A22*D22+3*A24+6*A12					[215]
$C_6Cl_4O_2$		2,3,5,6-tetrachloro-2,5-cyclohexadiene-1,4-dione					
	567.2	30.87	0	54.43	57.4	30.87	32.6
		A14+3*A15+2*A114+4*A19+4*A22*F22					[215]
$C_6Cl_5NO_2$		pentachloronitrobenzene					
	418	18.41	0	44.04	53.8	18.41	22.5
		6*A12+5*F22*A22+A50					[215]
C_6Cl_6		hexachlorobenzene					
	505	23.85	0	47.23	52.2	23.85	26.4
		6*F22*A22+6*A12					[215]
$C_6F_5NO_2$		pentafluoronitrobenzene					
	250.5	11.81	0	47.13	56.0	11.81	14.0
		5*A24+A50+6*A12					[216]
C_6F_6		hexafluorobenzene					
	278.3	11.59	0	41.67	54.9	11.59	15.3
		6*A24+6*A12					[216]
C_6F_{14}		*n*-perfluorohexane					
	103	0.97	10				
	185	6.84	36.82	46.82	74.0	7.8	13.7
		8*A26+6*A4*B4+6*A25					[216, 67]
$C_6F_{15}N$		perfluorotriethylamine					
	146.4	1.56	10.67				
	156.2	5.56	35.61	46.28	59.1	7.12	9.2
		6*A26+A43+6*A4*B4+9*A25					[216]
C_6N_4		tetracyanoethylene					
	472.2	24.92	0	52.77	49.5	24.92	23.4
		4*A56+2*A7					[3]
C_6HBr_5O		pentabromophenol					
	441.5	11.29	25.57				
	502	19.14	38.13	63.7	63.1	30.43	31.7
		6*A12+A31+5*A21					[191]
$C_6HCl_4NO_2$		1,2,4,5-tetrachloro-3-nitrobenzene					
	373.3	19.46	0	52.13	52.5	19.46	19.6
		4*E22*A22+A50+5*A12+A10					[215]
C_6HCl_5		pentachlorobenzene					
	357.7	20.6	0	57.59	50.9	20.6	18.2
		5*A12+5*A22*E22+A10					[215]

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_6HCl_5O		pentachlorophenol					
	462.5	17.15	0	37.08	56.3	17.15	26.0
		5*A22*F22+A31+6*A12					[215, 191]
C_6HF_5		pentafluorobenzene					
	225.7	10.88	0	48.24	53.2	10.88	12.0
		5*A24+5*A12+A10					[215]
C_6HF_5O		pentafluorophenol					
	287	1.16	4.04				
	310.6	16.41	52.83	56.87	58.5	17.57	18.2
		6*A12+A31+5*A24					[72]
$C_6H_2Br_4$		1,2,4,5-tetrabromobenzene					
	306.8	0.34	1.09				
	453.1	27.88	61.53	62.62	55.1	28.22	25.0
		4*A21+4*A12+2*A10					[216]
$C_6H_2Cl_4$		1,2,3,4-tetrachlorobenzene					
	320	17	0	53.13	49.6	17	15.9
		4*A12+2*A10+4*A22*D22					[215]
$C_6H_2Cl_4$		1,2,4,5-tetrachlorobenzene					
	421.2	24.1	0	57.22	49.6	24.1	20.9
		4*A12+2*A10+4*A22*D22					[215]
$C_6H_2Cl_4$		1,2,3,5-tetrachlorobenzene					
	323.9	19	0	58.66	49.6	19	16.1
		4*A12+2*A10+4*A22*D22					[215]
$C_6H_2Cl_5N$		pentachloroaniline					
	505.8	18.7	0	36.97	57.4	18.7	29.0
		6*A12+5*A22*F22+A45					[215]
$C_6H_2F_4$		1,2,3,4-tetrafluorobenzene					
	233.3	10.93	0	46.85	51.4	10.93	12.0
		4*A12+2*A10+4*A24					[65]
$C_6H_2F_4$		1,2,3,5-tetrafluorobenzene					
	226.9	10.67	0	47.01	51.4	10.67	11.7
		4*A12+2*A10+4*A24					[65]
$C_6H_2F_4$		1,2,4,5-tetrafluorobenzene					
	277	15.05	0	54.31	51.4	15.05	14.3
		4*A12+2*A10+4*A24					[65]
$C_6H_2F_5N$		pentafluoroaniline					
	287.4	3.94	13.71				
	306.8	14.27	46.51	60.22	59.6	18.21	18.3
		5*A24+A45+6*A12					[216]
$C_6H_3BrCl_2O$		4-bromo-2,5-dichlorophenol					
	343.4	22.11	0	64.39	55.0	22.11	18.9
		2*A10+4*A12+2*A22*D22+A21+A31					[221]
$C_6H_3Br_3O$		2,4,6-tribromophenol					
	366.2	18.52	0	50.57	57.8	18.52	21.2
		4*A12+2*A10+3*A21+A31					[215]
$C_6H_3Cl_3$		1,2,3-trichlorobenzene					
	326.9	20.5	0	62.71	48.4	20.5	15.8
		3*A10+3*A12+3*A22*C22					[215]
$C_6H_3Cl_3$		1,3,5-trichlorobenzene					
	336.7	18.2	0	54.05	48.4	18.2	16.3
		3*A10+3*A12+3*A22*C22					[215]
$C_6H_3Cl_3O$		2,4,5-trichlorophenol					
	340.3	21.59	0	63.44	53.7	21.59	18.3
		4*A12+2*A10+3*A22*D22+A31					[221]
$C_6H_3Cl_4N$		2-chloro-6-(trichloromethyl)pyridine					
	337.2	20.3	0	60.2	58.0	20.3	19.6
		3*A10+A41+A11+A12+A4*B4+4*A22*E22					[216]
$C_6H_3N_3O_6$		1,3,5-trinitrobenzene					
	370	1.9	5.13				
	380.3	14.8	38.95	44.08	53.0	16.71	20.2
		3*A10+3*A12+3*A50*C50					[216]
$C_6H_3N_3O_7$		picric acid					
	394.1	17.1	0	43.39	58.4	17.1	23.0
		2*A10+4*A12+3*A50+A31					[216]
$C_6H_3N_3O_8$		2,4,6-trinitroresorcinol					
	454.8	33.5	0	73.66	63.7	33.5	29.0
		A10+5*A12+2*A31+3*A50					[216]
C_6H_4BrCl		1,2-bromochlorobenzene					

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)
	260.6	12.37	0	47.47	48.4	12.37	12.6
		A22*B22+A21+2*A12+4*A10					[216]
C_6H_4BrCl		1,3-bromochlorobenzene					
	252.0	12.29	0	48.77	48.4	12.29	12.2
		A22*B22+A21+2*A12+4*A10					[216]
C_6H_4BrCl		1,4-bromochlorobenzene					
	337.8	18.76	0	55.54	48.4	18.76	16.4
		A22*B22+A21+2*A12+4*A10					[216]
C_6H_4BrI		1,2-bromoiodobenzene					
	294.2	14.42	0	49.01	51.6	14.42	15.2
		4*A10+2*A12+A21+A29					[215]
C_6H_4BrI		1,3-bromoiodobenzene					
	282.5	12.16	0	43.04	51.6	12.16	14.6
		4*A10+2*A12+A21+A29					[215]
C_6H_4BrI		1,4-bromoiodobenzene					
	363.3	19.13	0	52.66	51.6	19.13	18.8
		4*A10+2*A12+A21+A29					[215]
$C_6H_4Br_2$		1,2-dibromobenzene					
	275	12.61	0	45.58	49.8	12.61	13.7
		4*A10+2*A12+2*A21					[215]
$C_6H_4Br_2$		1,3-dibromobenzene					
	266.3	13.21	0	49.61	49.8	13.21	13.3
		4*A10+2*A12+2*A21					[215]
$C_6H_4Br_2$		1,4-dibromobenzene					
	360.1	20.04	0	55.65	49.8	20.04	17.9
		2*A21+4*A10+2*A12					[215]
$C_6H_4Br_2O$		2,4-dibromophenol					
	313	14.64	0	46.79	55.2	14.64	17.3
		3*A10+3*A12+2*A21+A31					[215]
$C_6H_4ClNO_2$		1,2-chloronitrobenzene					
	308.2	19.08	0	61.9	48.6	19.08	15.0
		4*A10+2*A12+A22*B22+A50					[228]
$C_6H_4ClNO_2$		1,4-nitrochlorobenzene					
	354.6	11.85	0	33.42	48.6	11.85	17.2
		4*A10+2*A12+A50+A22*B22					[216]
$C_6H_4ClNO_2$		1,3-nitrochlorobenzene					
	317.6	19.37	0	60.99	48.6	19.37	15.4
		A22*B22+A50+4*A10+2*A12					[215]
$C_6H_4Cl_2$		1,2-dichlorobenzene					
	256.5	12.93	0	50.41	47.1	12.93	12.1
		4*A10+2*A12+2*A22*B22					[215]
$C_6H_4Cl_2$		1,3-dichlorobenzene					
	248.4	12.64	0	50.89	47.1	12.64	11.7
		4*A10+2*A12+2*A22*B22					[215]
$C_6H_4Cl_2$		1,4-dichlorobenzene					
	326	18.16	0	55.65	47.1	18.16	15.3
		2*A22*B22+4*A10+2*A12					[215]
$C_6H_4Cl_2N_2O_2$		2,6-dichloro-4-nitroaniline					
	466.8	32.64	0	69.92	56.4	32.64	26.3
		4*A12+2*A10+A45+2*A22*D22+A50					[215]
$C_6H_4Cl_2O$		2,3-dichlorophenol					
	330	21.36	0	64.73	52.4	21.36	17.3
		3*A10+3*A12+A31+2*A22*C22					[215]
$C_6H_4Cl_2O$		2,4-dichlorophenol					
	318	20.09	0	63.18	52.4	20.09	16.7
		3*A10+3*A12+A31+2*A22*C22					[216]
$C_6H_4Cl_2O$		2,5-dichlorophenol					
	331	22.43	0	67.76	52.4	22.43	17.4
		3*A10+3*A12+A31+2*A22*C22					[216]
$C_6H_4Cl_2O$		2,6-dichlorophenol					
	340	22.14	0	65.12	52.4	22.14	17.8
		3*A10+3*A12+A31+2*A22*C22					[216]
$C_6H_4Cl_2O$		3,4-dichlorophenol					
	341	20.93	0	61.38	52.4	20.93	17.9
		3*A10+3*A12+A31+2*A22*C22					[216]
$C_6H_4Cl_2O$		3,5-dichlorophenol					
	341	20.51	0	60.15	52.4	20.51	17.9
		3*A10+3*A12+A31+2*A22*C22					[216]
$C_6H_4F_2$		1,2-difluorobenzene					

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)
	226	11.05 4*A10+2*A12+2*A24	0	48.95	48.0	11.05	10.8 [216]
$C_6H_4F_2$		1,3-difluorobenzene					
	186.8	0.83	4.43				
	204.0	8.58 2*A24+2*A12+4*A10	42.05	46.48	48.0	9.4	9.8 [216]
$C_6H_4I_2$		1,2-diiodobenzene					
	296.6	14.01 2*A29+2*A12+4*A10	0	47.24	53.5	14.01	15.9 [215]
$C_6H_4I_2$		1,3-diiodobenzene					
	307.4	15.93 2*A29+2*A12+4*A10	0	51.82	53.5	15.93	16.4 [215]
$C_6H_4I_2$		1,4-diiodobenzene					
	402	22.37 2*A29+2*A12+4*A10	0	55.65	53.5	22.37	21.5 [215]
$C_6H_4N_2O_4$		1,2-dinitrobenzene					
	396.1	22.84 4*A10+2*A12+2*A50	0	57.66	50.2	22.84	19.9 [216]
$C_6H_4N_2O_4$		1,3-dinitrobenzene					
	363.2	17.36 4*A10+2*A12+2*A50	0	47.82	50.2	17.36	18.2 [215]
$C_6H_4N_2O_4$		1,4-dinitrobenzene					
	446.7	28.12 4*A10+2*A12+2*A50	0	62.93	50.2	28.12	22.4 [215]
$C_6H_4N_2O_5$		2,3-dinitrophenol					
	417	26.24 3*A10+3*A12+2*A50+A31	0	62.93	55.5	26.24	23.2 [216]
$C_6H_4N_2O_5$		2,4-dinitrophenol					
	388	24.17 3*A10+3*A12+2*A50+A31	0	62.29	55.5	24.17	21.6 [216]
$C_6H_4N_2O_5$		2,5-dinitrophenol					
	381	23.73 3*A10+3*A12+2*A50+A31	0	62.28	55.5	23.73	21.2 [216]
$C_6H_4N_2O_5$		2,6-dinitrophenol					
	336	19.58 3*A10+3*A12+2*A50+A31	0	58.27	55.5	19.58	18.7 [216]
$C_6H_4N_2O_5$		3,4-dinitrophenol					
	407	25.37 3*A10+3*A12+2*A50+A31	0	62.33	55.5	25.37	22.6 [216]
$C_6H_4O_2$		*p*-benzoquinone					
	388	18.45 3*A15+A14+4*A18*B18+2*A114	0	47.56	29.4	18.45	11.4 [215]
C_6H_5Br		bromobenzene					
	242.4	10.7 5*A10+A12+A21	0	44.2	47.1	10.7	11.4 [216]
C_6H_5BrO		4-bromophenol					
	336	16.57 A21+4*A10+2*A12+A31	0	49.32	52.5	16.57	17.6 [216]
C_6H_5Cl		chlorobenzene					
	227.9	9.55 5*A10+A22+A12	0	41.92	40.4	9.55	9.2 [216]
C_6H_5ClO		2-chlorophenol					
	276	0.09	0.33				
	283	12.52 4*A10+2*A12+A22*B22+A31	44.24	44.57	51.2	12.61	14.5 [215]
C_6H_5ClO		3-chlorophenol					
	305.8	14.91 4*A10+2*A12+A22*B22+A31	0	48.76	51.2	14.91	15.6 [215]
C_6H_5ClO		4-chlorophenol					
	315.9	14.07 4*A10+2*A12+A22*B22+A31	0	44.54	51.2	14.07	16.2 [215]
$C_6H_5Cl_2N$		2,6-dichloro-4-benzenamine					
	467.2	29.48 3*A10+3*A12+2*A22*C22+A45	0	63.11	53.5	29.48	25.0 [221]
$C_6H_5Cl_3Si$		phenyltrichlorosilane					
	233.4	11.66 5*A10+A11+3*A22*D22+A109	0	49.96	48.9	11.66	11.4 [216]
C_6H_5F		fluorobenzene					

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)
	230.9	11.31	0	48.95	46.2	11.31	10.7
		5*A10+A12+A24					[250]
C_6H_5I		iodobenzene					
	241.8	9.75	0	40.31	49.0	9.75	11.8
		5*A10+A12+A29					[216]
$C_6H_5NO_2$		picolinic acid					
	411	30	0	72.99	49.2	30	20.2
		4*A10+A12+A41+A36*B36					[216]
$C_6H_5NO_2$		nicotinic acid					
	452	0.78	1.73				
	510	26.7	52.35	54.08	49.2	27.48	25.1
		4*A10+A12+A41+A36*B36					[182]
$C_6H_5NO_2$		isonicotinic acid					
	593	135	0	227.66	49.2	135	29.2
		4*A10+A12+A41+A36*B36					[216]
$C_6H_5NO_2$		nitrobenzene					
	278.8	12.12	0	43.5	47.3	12.12	13.2
		5*A10+A12+A50					[216]
$C_6H_5NO_3$		*o*-nitrophenol					
	318.2	17.45	0	54.83	52.7	17.45	16.8
		4*A10+2*A12+A50+A31					[215,188]
$C_6H_5NO_3$		*m*-nitrophenol					
	371.2	19.19	0	51.7	52.7	19.19	19.6
		4*A10+2*A12+A50+A31					[215,188]
$C_6H_5NO_3$		*p*-nitrophenol					
	388.2	18.25	0	47.02	52.7	18.25	20.5
		4*A10+2*A12+A50+A31					[216,188]
C_6H_6		benzene					
	278.7	9.87	0	35.4	44.5	9.87	12.4
		6*A10					[216]
$C_6H_6Cl_6$		1α,2α,3β,4α,5α,6β-hexachlorocyclohexane					
	386.8	22.13	0	57.23	53.2	22.13	20.6
		A14+3*A15+6*A16+6*A22*F22					[221]
$C_6H_6Cl_6$		1α,2α,3β,4α,5α,6β-hexachlorocyclohexane (lindane)					
	388.9	15.9	0	40.88	53.2	15.9	20.7
		A14+3*A15+6*A16+6*A22*F22					[221]
$C_6H_6N_2O_2$		2-nitroaniline					
	342.5	16.11	0	47.0	53.8	16.11	18.5
		4*A10+A45+A50+2*A12					[216]
$C_6H_6N_2O_2$		3-nitroaniline					
	387	23.68	0	61.16	53.8	23.68	20.8
		4*A10+A45+A50+2*A12					[216]
$C_6H_6N_2O_2$		4-nitroaniline					
	420.7	21.09	0	50.1	53.8	21.09	22.6
		4*A10+A45+A50+2*A12					[216]
$C_6H_6N_6O_{14}$		2,2,2-trinitroethyl 4,4,4-trinitrobutyrate					
	362.7	25.94	71.52				
	366.5	6.69	18.27	89.79	89.7	32.64	32.9
		3*A2+2*A4*B4+A38+6*A50					[122]
C_6H_6O		phenol					
	314	11.51	0	36.82	49.9	11.51	15.7
		5*A10+A31+A12					[216]
$C_6H_6O_2$		1,4-dihydroxybenzene					
	445	26.48	0	59.5	59.5	26.48	25.0
		4*A10+2*A31+2*A12					[199]
$C_6H_6O_2$		1,2-dihydroxybenzene					
	376.9	22.01	0	58.39	55.2	22.01	20.8
		4*A10+2*A31+2*A12					[199]
$C_6H_6O_2$		1,3-dihydroxybenzene					
	366.8	1.2	3.27				
	382.6	18.9	49.41	52.64	55.2	20.1	21.1
		4*A10+2*A31+2*A12					[199]
$C_6H_6O_3$		1,2,3-trihydroxybenzene					
	407.2	18.55	0	45.56	60.6	18.55	24.7
		3*A10+3*A12+3*A31					[4]
C_6H_6S		thiophenol					
	258.3	11.4	0	44.3	52.6	11.3	13.6
		5*A10+A12+A86					[281]
C_6H_7N		aniline					

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)
	267.1	10.54	0	39.45	51.0	10.54	14.1
		5*A10+A12+A45					[216]
C_6H_7N		2-methylpyridine					
	206.5	9.72	0	47.1	48.5	9.72	10.0
		4*A10+A11+A1+A41					[216]
C_6H_7N		3-methylpyridine					
	255	14.18	0	55.62	48.5	14.18	12.4
		4*A10+A11+A1+A41					[216]
C_6H_7NO		*o*-aminophenol					
	447.4	34	0	75.99	56.3	34	25.2
		4*A10+2*A12+A31+A45					[216]
C_6H_7NO		*m*-aminophenol					
	399	22.98	0	57.59	56.3	22.98	22.5
		4*A10+2*A12+A31+A45					[139]
C_6H_7NO		*p*-aminophenol					
	459.5	31.2	0	67.9	56.3	31.2	25.9
	462.5	26	0	56.22	56.3	26.0	26.0
		4*A10+2*A12+A31+A45					[216,223]
C_6H_8		1,3-cyclohexadiene					
	161	4.2	0	26.1	38.0	4.2	6.1
		A14+3*A15+4*A18					[216]
C_6H_8		1,4-cyclohexadiene					
	192	0.82	4.25				
	224	5.72	25.51	29.76	38.0	6.53	8.5
		A14+3*A15+4*A18					[216]
$C_6H_8N_2$		*o*-phenylenediamine					
	373.9	23.1	0	61.78	57.43	23.1	21.47
		4*A10+2*A12+2*A45					[216]
$C_6H_8N_2$		*m*-phenylenediamine					
	335.5	15.4	0	45.9	57.43	15.4	19.27
		4*A10+2*A12+2*A45					[216]
$C_6H_8N_2$		*p*-phenylenediamine					
	412.3	21.7	0	52.63	57.43	21.7	23.68
		4*A10+2*A12+2*A45					[216]
$C_6H_8N_2$		phenylhydrazine					
	292.8	16.43	0	56.11	45.7	16.43	13.4
		5*A10+A12+A45+A44					[215]
$C_6H_8N_2O_2$		N-acetylglycine amide					
	408.2	25.6	0	62.71	54.1	25.6	22.1
		A1+A60+A2+A61					[278]
$C_6H_8N_2O_2$		1,3-dimethyluracil					
	398	14.6	0	36.68	30.0	14.6	11.9
		2*A1+A14+3*A15+2*A125+2*A18*B18					[292]
$C_6H_8N_4O_2$		*bis*(2-cyanoethyl)-N-nitroamine					
	327	44.99	0	137.57	109.1	44.99	35.7
		4*A2+2*A56+A51+A47					[225]
$C_6H_8O_2$		1,4-cyclohexanedione					
	322.2	6.15	19.09				
	339.2	0.96	2.83				
	348.2	10.04	28.84	50.76	41.8	17.15	14.5
		3*A15+A14+2*A114					[114]
$C_6H_8O_4$		dimethyl maleate					
	254	14.64	0	57.74	58.4	14.64	14.8
		2*A1+2*B6*A6+2*A38					[216]
$C_6H_8O_4$		dimethyl fumarate					
	375	35.15	0	93.72	58.4	35.15	21.9
		2*A1+2*A38+2*B6*A6					[216]
$C_6H_8O_4$		DL 3,6-dimethyl-1,4-dioxane-2,5-dione					
	397.5	24.7	0	62.14	49.1	24.7	19.5
		A14+A15+2*A115+2*A16+2*A1					[216]
C_6H_8S		2,5-dimethylthiophene					
	210.6	8.91	0	42.31	51.1	8.91	10.8
		2*A1+A131+A14+2*A15+2*A19+2*A18					[216]
$C_6H_8ClO_2$		chloroethyl methacrylate					
	235.1	17	0	72.31	62.3	17	14.7
		2*A2+A22*B22+A5+A7+A1+A38					[216]
C_6H_9N		2,4-dimethylpyrrole					
	268.5	9.6	0	35.75	48.9	9.6	13.1

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)
		*A*14+2**A*15+*A*18+2**A*1+*A*121+*A*18**B*18+2**A*19					[70]
C_6H_9N		2,5-dimethylpyrrole					
	280.9	9.3	0	33.09	50.4	9.3	14.2
		*A*14+2**A*15+2**A*18+2**A*1+*A*121+2**A*19					[216]
C_6H_9NS		2,4,5-trimethylthiazole					
	240.7	9	0	37.39	60.2	9	14.5
		*A*14+2**A*15+3**A*19+3**A*1+*A*118+*A*131					[61]
C_6H_{10}		cyclohexane					
	138.7	4.23	30.5				
	169.7	3.28	19.35	49.85	41.3	7.51	7.0
		*A*14+3**A*15+2**A*18					[216]
$C_6H_{10}N_2O$		2,3-diazabicyclo[2.2.2]oct-2-ene N-oxide					
	359.3	5.02	13.97				
	399.3	8.05	20.16				
	438	3.84	8.77	42.9	47.6	16.91	20.8
		2**A*14+2**A*15+2**A*16+*A*123					[42]
$C_6H_{10}O$		cyclohexanone					
	220.8	8.66	39.22				
	245.2	1.33	5.42	44.64	43.1	9.99	10.6
		*A*14+3**A*15+*A*114					[156]
$C_6H_{10}O$		cyclohexene oxide					
	193.1	9.54	49.38				
	238.1	1.06	4.47	53.85	42.2	10.6	10.1
		2**A*14+*A*15+*A*112+2**A*16					[156]
$C_6H_{10}O_2$		ε-caprolactone					
	272	13.82	50.81	50.79	51.3	13.82	14.0
		*A*14+4**A*15+*A*115					[32]
$C_6H_{10}O_3$		2,2-dimethyltrimethylene carbonate					
	324.1	10.3	31.78				
	387.2	5.62	14.52	46.31	46.3	15.92	17.9
		*A*14+3**A*15+*A*116+2**A*1+*A*17					[200]
$C_6H_{10}O_4$		adipic acid					
	426.4	34.85	0	81.73	69.6	34.85	29.7
		4**A*2**B*2+2**A*36**B*36					[340]
$C_6H_{10}O_6$		(*dl*) dimethyl tartrate					
	360.2	26.94	0	74.81	76.7	26.94	27.6
		2**A*38+2**A*3**B*3+2**A*1+2**A*30**D*30					[220]
$C_6H_{10}O_6$		(*d*) dimethyl tartrate					
	322.2	17.36	0	53.89	76.7	17.36	24.7
		2**A*38+2**A*3**B*3+2**A*1+2**A*30**D*30					[220]
$C_6H_{11}Br$		bromocyclohexane					
	216.9	10.79	0	49.75	47.3	10.79	10.3
		*A*14+3**A*15+*A*21+*A*16					[190]
$C_6H_{11}Cl$		chlorocyclohexane					
	120	0.05	0.42				
	220.4	8.01	36.35				
	229.3	2.04	8.91	45.67	40.5	10.1	9.3
		*A*14+3**A*15+*A*16+*A*22					[229]
$C_6H_{11}NO$		cyclohexanone oxime					
	240.8	0.01	0.06				
	362.6	12.7	35.02				
	273.4	0.09	0.34	35.43	45.8	12.81	12.5
		*A*14+3**A*15+*A*19+*A*53					[5]
$C_6H_{11}NO$		ε-caprolactam					
	343.3	16.1	0	46.89	50.9	16.1	17.5
		*A*14+4**A*15+*A*124					[6]
$C_6H_{11}NO_3$		N-dimethylaminosuccinamic acid					
	431.4	36.97	0	85.71	54.4	36.97	23.5
		2**A*1+2**A*2+*A*36**B*36+*A*59					[221]
$C_6H_{11}N_2O_3PS_2$		S-2,3-dihydro-5-methoxy-2-oxo-1,3,4-thiadiazol-3-ylmethyl O,O-dimethyl phosphorodithioate					
	315.1	28.54	0	90.59	90.7	28.54	28.6
		3*A1+A14+2*A15+A138+A19+A118+*A*32+*A*80					[221]
C_6H_{12}		cyclohexane					
	186.1	6.74	36.2				
	279.8	2.68	9.57	45.77	44.5	9.41	12.5
		*A*14+3**A*15					[216]
C_6H_{12}		methylcyclopentane					
	130.7	6.93	0	53.01	43.6	6.93	5.7
		*A*14+*A*16+*A*1+2**A*15					[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_6H_{12}		1-hexene					
	133.4	9.35	0	70.1	61.6	9.37	8.2
		$A1+3*A2+A5+A6$					[216]
C_6H_{12}		2,3-dimethyl-2-butene					
	196.8	3.53	17.94				
	198.9	6.44	32.39	50.34	48.9	9.97	9.6
		$4*A1+2*A7$					[216]
C_6H_{12}		3,3-dimethyl-1-butene					
	124.9	4.35	34.84				
	158.4	1.09	6.87	41.71	40.5	5.44	5.1
		$A4+3*A1+A5+A6$					[216]
C_6H_{12}		*cis*-2-hexene					
	132	8.88	0	67.27	59.9	8.88	7.9
		$2*A1+2*A2+2*A6$					[165]
$C_6H_{12}N_2$		1,4-diazabicyclo[2.2.2]octane					
	351.1	10.54	30.08				
	433	7.45	17.15	47.24	35.6	18.0	15.4
		$2*A14+2*A15+2*A119$					[216]
$C_6H_{12}N_2O_3$		β-alanyl-β-alanine					
	480.1	58.3	0	121.45	81.4	58.3	39.1
		$4*A2+A45+A36*C36+A60$					[216]
$C_6H_{12}N_2O_3$		α-alanyl-α-alanine (DL)					
	483.2	33.2	0	68.72	68.4	33.2	33.0
		$2*A1+A45+A36*C36+A60+2*A3*B3$					[216]
$C_6H_{12}O$		cyclohexanol					
	265.5	8.8	33.3				
	299.1	1.8	6.0	39.3	31.5	9.9	9.4
		$A14+3*A15+A16+A30$					[81]
$C_6H_{12}O$		1-methylcyclopentanol					
	310.2	8.41	0	27.11	25.5	8.41	7.9
		$A14+2*A15+A1+A17+A30$					[230]
$C_6H_{12}O$		hexanal					
	214.9	13.3	61.89				
	243.2	0.34	1.38	63.27	76.4	13.64	18.6
		$A14+4*A2*B2+A34$					[128, 168]
$C_6H_{12}O$		3,3-dimethyl-2-butanone					
	221.7	11.34	0	51.04	52.0	11.34	11.5
		$4*A1+A4*B4+A35$					[216]
$C_6H_{12}O$		3-hexanone					
	145	0.68	4.7				
	217.7	13.47	61.89	66.61	61.1	14.15	13.3
		$2*A1+3*A2+A35$					[216]
$C_6H_{12}O$		2-hexanone					
	217.7	14.9	68.42	68.41	61.1	14.9	13.3
		$2*A1+3*A2+A35$					[216]
$C_6H_{12}O_2$		2,2-dimethyl-1,3-dioxane					
	229.6	12.1	0	52.7	47.5	12.1	10.9
		$A14+3*A15+2*A1+A17+2*A112$					[47]
$C_6H_{12}O_2$		*cis*-1,2-cyclohexanediol					
	360.4	19.89	55.19				
	371.6	3.32	8.93	64.12	51.2	23.21	19.0
		$A14+3*A15+2*A30*B30+2*A16$					[204]
$C_6H_{12}O_2$		*trans*-1,2-cyclohexanediol					
	372.3	18.51	0	49.72	51.2	18.51	19.1
		$A14+3*A15+2*A30*B30+2*A16$					[204]
$C_6H_{12}O_3$		2,4,6-trimethyl-1,3,5-trioxane					
	142.7	0.26	1.81				
	147.5	0.77	5.24				
	285.7	13.52	47.32	54.37	56.7	14.55	16.2
		$3*A1+3*A16+A14+3*A15+3*A112$					[216]
$C_6H_{12}O_6$		α-D-glucose					
	414	31.42	0	75.9	93.0	31.42	38.5
		$A14+3*A15+5*A30*F30+A2+5*A16+A112$					[216]
$C_6H_{12}O_6$		myo-inositol					
	496.9	47.9	0	96.4	92.7	47.9	46.1
		$A14+3*A15+6*A16+6*A30*F30$					[216]
$C_6H_{12}S$		cyclopentyl methyl sulfide					
	165	0.9	5.44				
	169.9	9.2	54.31	59.75	45.7	10.1	7.8
		$A14+2*A15+A1+A84+A16$					[105]

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)
$C_6H_{12}S$		cyclohexanethiol					
	189.6	10	0	52.72	52.8	10.0	10.0
		A14+3*A15+A86+A16					[341]
$C_6H_{13}Br$		1-bromohexane					
	188.1	18.05	0	95.98	81.8	18.05	15.4
		A1+5*A2*B2+A21					[216]
$C_6H_{13}N$		2-methylpiperidine					
	269.4	18.58	0	68.99	49.5	18.58	13.3
		A14+3*A15+A121+A1+A16					[216]
$C_6H_{13}NO$		hexanamide					
	374	25.1	0	67.12	82.8	25.1	31.0
		4*A2*B2+A1+A61					[279]
C_6H_{14}		*n*-hexane					
	177.8	13.08	0	73.22	72.5	13.08	12.9
		2*A1+4*A2*B2					[216]
C_6H_{14}		2,3-dimethylbutane					
	136.1	6.43	47.22				
	107	2.37	22.13				
	145.2	0.79	5.47	52.96	37.6	9.59	5.1
		4*A1+2*A3					[216]
C_6H_{14}		3-methylpentane					
	110.3	5.31	0	48.17	50.6	5.31	5.6
		2*A2+3*A1+A3					[216]
C_6H_{14}		2-methylpentane					
	119.6	6.27	0	52.43	50.6	6.27	6.05
		2*A2+3*A1+A3					[216]
C_6H_{14}		2,2-dimethylbutane					
	126.8	5.4	42.57				
	140.8	0.28	2.02				
	174.3	0.58	3.31	45.88	42.6	6.26	7.4
		4*A1+A2+A4					[216]
$C_6H_{14}O$		1-hexanol					
	225.8	15.48	0	68.56	66.0	15.48	14.9
		A1+5*A2*B2+A30					[216]
$C_6H_{14}O$		isopropyl ether					
	187.8	12.05	0	64.02	55.7	12.05	10.5
		4*A1+2*A3*B3+A32					[66]
$C_6H_{14}O$		4-oxaheptane					
	158.4	10.77	0	67.99	68.4	10.77	10.8
		2*A1+4*A2+A32					[216]
$C_6H_{14}O_2$		2,3-dimethyl-2,3-butanediol					
	316.2	14.7	0	46.49	60.8	14.7	19.2
		4*A1+2*A4*B4+2*B30*A30					[231]
$C_6H_{14}O_2$		1,6-hexanediol					
	320.6	25.52	0	79.6	92.2	25.52	29.0
		2*A30*B30+6*A2*B2					[216]
$C_6H_{14}O_3$		2,5,8-trioxanonane					
	209.1	17.8	0	85.1	77.8	17.8	16.3
		2*A1+4*A2+3*A32					[216]
$C_6H_{14}O_6$		D sorbitol					
	366.5	30.2	0	82.4	111.7	30.2	40.9
		2*A2+4*A3*B3+6*A30*F30					[216]
$C_6H_{14}O_6$		dulcitol					
	460.3	65.1	0	141.4	111.7	65.1	51.4
		2*A2+4*A3*B3+6*A30*F30					[216]
$C_6H_{14}O_6$		D mannitol					
	439.1	56.1	0	127.8	111.7	56.1	49.0
	438.7	50.6	0	115.3	111.7	50.6	49.0
		2*A2+4*A3*B3+6*A30*F30					[216, 394]
$C_6H_{14}S$		diisopropyl sulfide					
	195.1	10.42	0	53.39	52.8	10.42	10.4
		4*A1+2*A3*B3+A84					[341]
$C_6H_{14}S$		dipropyl sulfide					
	170.4	12.14	0	71.25	65.8	12.14	11.2
		2*A1+4*A2+A84					[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)	
$C_6H_{14}S$		butyl ethyl sulfide						
	178.1	12.39	0	69.57	65.8	12.39	11.7	
		$2*A1+4*A2+A84$					[136]	C_7
$C_6H_{14}S$		1-hexanethiol						
	192.6	18.03	0	93.51	87.2	18.03	16.8	
		$5*A2*B2+A1+A86$					[216]	C_7
$C_6H_{14}S_2$		dipropyl disulfide						
	187.7	13.81	0	73.55	73.3	13.81	13.8	
		$2*A1+4*A2+A85$					[216]	C_7
$C_6H_{15}Al$		triethylaluminum						
	225	10.6	0	47.11	49.5	10.6	11.1	
		$3*A1+3*A2+A97$					[216]	C_7
$C_6H_{15}As$		triethylarsine						
	181.8	11.06	0	60.83	67.7	11.06	12.3	
		$3*A1+3*A2+A98$					[216]	C
$C_6H_{15}B$		triethylborane						
	180.3	11.85	0	65.7	57.0	11.85	10.3	
		$3*A1+3*A2+A99$					[216]	C
$C_6H_{15}Bi$		triethylbismuth						
	145.8	8.7	0	59.64	59.7	8.7	8.7	
		$3*A1+3*A2+A100$					[167]	C
$C_6H_{15}Ga$		triethylgallium						
	193.5	11.64	0	60.18	62.2	11.64	12.0	
		$3*A1+3*A2+A101$					[216]	C
$C_6H_{15}In$		triethylindium						
	237.6	13.01	0	54.76	54.8	13.01	13.0	
		$3*A1+3*A2+A105$					[216]	C
$C_6H_{15}Sb$		triethylantimony						
	153.9	9.45	0	61.42	61.4	9.45	9.5	
		$3*A1+3*A2+A107$					[216]	C
$C_6H_{16}Si_2$		1,1,3,3-tetramethyl-1,3-disilacyclobutane						
	266	10.26	0	38.57	38.0	10.26	10.1	
		$A14+A15+2*A139+4*A1$					[216]	C
$C_6H_{18}OSi_2$		hexamethyldisiloxane						
	204.9	11.92	0	58.17	56.0	11.92	11.5	
		$6*A1+A32*B32+2*A109$					[216]	C
$C_6H_{18}O_3Si_3$		hexamethylcyclotrisiloxane						
	335.2	16.61	0	49.55	49.6	16.61	16.6	
		$A14+3*A15+6*A1+3*A112+3*A139$					[216,121]	C
$C_6H_{18}Si_2$		hexamethyldisilane						
	221.8	9.75	43.95					
	287.7	3.02	10.49	54.44	51.3	12.77	14.8	
		$6*A1+2*A109$					[216]	C
$C_6H_{21}N_3Si_3$		hexamethylcyclotrisilazane						
	254.4	15.17	0	59.63	52.4	15.17	13.3	
		$A14+3*A15+3*A139+6*A1+3*A121$					[216]	C
C_7F_8		perfluorotoluene						
	207	11.49	0	55.23	53.0	11.49	11.0	
		$5*A12+A11+A4*B4+5*A24+3*A25$					[216]	C
C_7F_{16}		perfluoroheptane						
	180.4	6.67	36.97					
	221.9	6.95	31.31	68.28	83.1	13.62	18.5	
		$7*A4*B4+6*A25+10*A26$					[216,67]	C
$C_7H_3Br_2NO$		3,5-dibromo-4-hydroxybenzonitrile						
	464	32.03	0	69.03	58.0	32.03	26.9	
		$2*A21+A56+A31+4*A12+2*A10$					[221]	
$C_7H_3F_5$		2,3,4,5,6-pentafluorotoluene						
	243.7	13.28	0	54.48	53.7	13.28	13.1	
		$5*A12+A11+A1+5*A24$					[216,77]	
$C_7H_3Cl_2N$		2,6-dichlorobenzonitrile						
	417.2	26.17	0	62.73	49.9	26.17	20.8	
		$2*A22*C22+A56+3*A12+3*A10$					[215]	
$C_7H_3Cl_3O_2$		2,3,6-trichlorobenzoic acid						
	402.7	23.85	0	59.23	63.5	23.85	25.6	
		$4*A12+2*A10+3*A22*D22+A36*D36$					[215]	
$C_7H_3I_2NO$		4-hydroxy-3,5-diiodobenzonitrile						
	482.9	33.63	0	69.64	61.7	33.63	29.8	
		$4*A12+2*A10+2*A29+A56+A31$					[221]	
$C_7H_3I_3O_2$		2,3,5-triiodobenzoic acid						

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)
	503.8	32.23	0	63.97	73.1	32.23	36.8 [215]
		3*A29+A36*D36+4*A12+2*A10					
$C_7H_4Cl_2O_2$		3,5-dichlorobenzoic acid					
	459.3	22.97	0	50.01	62.2	22.97	28.6 [215]
		3*A12+3*A10+2*A22*C22+A36*C36					
$C_7H_4Cl_3NO_3$		3,5,6-trichloro-2-pyridinyloxyacetic acid					
	423.3	31.17	0	73.63	78.8	31.17	33.4 [221]
		A10+4*A12+3*A22*F22+A41+A32+A36*F36+A2					
$C_7H_4N_2O_6$		3,5-dinitrobenzoic acid					
	480.4	22.8	0	47.47	65.3	22.8	31.4 [280]
		3*A12+2*A50+A36*C36+3*A10					
$C_7H_5Cl_3N_2O_2$		methyl 4-amino-3,5,6-trichloro-2-picolinate					
	394.3	26.78	0	67.91	68.7	26.78	27.1 [232]
		5*A12+A41+A38+3*A22*F22+A45+A1					
$C_7H_5ClO_2$		2-chlorobenzoic acid					
	413.4	25.73	0	62.34	47.0	25.73	19.4 [215]
		4*A10+A36*B36+2*A12+A22*B22					
$C_7H_5ClO_2$		3-chlorobenzoic acid					
	427.4	23.85	0	55.65	47.0	23.85	20.1 [215]
		4*A10+A36*B36+2*A12+A22*B22					
$C_7H_5ClO_2$		4-chlorobenzoic acid					
	512.9	32.26	0	62.76	47.0	32.26	24.1 [215]
		4*A10+A36*B36+2*A12+A22*B22					
$C_7H_5Cl_2NO_2$		3-amino-2,5-dichlorobenzoic acid					
	475.6	37.42	0	78.68	68.7	37.42	32.7 [215]
		2*A22*D22+A45+A36*D36+4*A12+2*A10					
$C_7H_5Cl_3$		benzotrichloride					
	236.0	13.95	0	59.11	53.2	13.95	12.6 [216]
		5*A10+A11+3*A22*C22+A4*B4					
$C_7H_5F_3$		benzotrifluoride					
	244.1	13.78	0	56.45	44.7	13.77	10.9 [216]
		5*A10+A11+A4*B4+3*A25					
$C_7H_5IO_2$		2-iodobenzoic acid					
	435.1	21.38	0	49.14	50.2	21.38	21.8 [7]
		4*A10+2*A12+A36*B36+A29					
$C_7H_5IO_2$		3-iodobenzoic acid					
	460.4	28.7	0	62.34	50.2	28.7	23.1 [7]
		4*A10+2*A12+A36*B36+A29					
$C_7H_5IO_2$		4-iodobenzoic acid					
	543.8	35.24	0	64.8	50.2	35.24	27.3 [7]
		4*A10+2*A12+A36*B36+A29					
C_7H_5N		benzonitrile					
	260.3	10.98	0	42.18	47.3	10.98	12.3 [134]
		5*A10+A12+A56					
C_7H_5NO		benzoxazole					
	247	0.02	0.07				
	302.5	16.78	55.48	55.56	44.6	16.8	13.5 [216]
		A14+2*A15+2*A19+A18*B18+A112+A118+4*A10					
$C_7H_5NO_4$		*o*-nitrobenzoic acid					
	419	27.99	0	66.8	48.5	27.99	20.3 [216]
		4*A10+2*A12+A36*B36+A50					
$C_7H_5NO_4$		*m*-nitrobenzoic acid					
	414.3	19.33	0	46.66	48.5	19.33	20.1 [216]
		4*A10+2*A12+A50+A36*B36					
$C_7H_5NO_4$		*p*-nitrobenzoic acid					
	512.4	36.9	0	72.02	48.5	36.9	24.9 [215]
		4*A10+2*A12+A36*B36+A50					
C_7H_5NS		benzothiazole					
	275.6	12.8	0	46.36	46.2	12.8	12.7 [216]
		4*A10+A14+2*A15+A118*+2*A19+A131+A18*B18					
$C_7H_5N_3O_6$		2,4,5-trinitrotoluene					
	376.2	24.7	0	66.0	53.5	24.7	20.1 [216]
		2*A10+3*A12+3*A50*C50+A1+A11					
$C_7H_5N_3O_6$		2,4,6-trinitrotoluene					
	352.2	23.43	0	66.52	53.5	23.43	18.9 [217]
		2*A10+3*A12+3*A50*C50+A1+A11					
$C_7H_5N_5O_8$		N-methyl-2,4,6,N-tetranitroaniline					
	402.6	25.86	0	64.23	100.8	25.86	40.6 [216]
		4*A12+3*A50+A51+A1+2*A10+A47					

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)
$C_7H_6N_2$	443.2	benzimidazole 19.25 4*A10+A118+A121+A14+2*A15+2*A19+A18*B18	0	43.43	45.5	19.25	20.2 [282]
$C_7H_6N_2O_4$	343.3	2,4-dinitrotoluene 20.12 3*A10+A11+2*A12+2*A50+A1	0	58.61	50.7	20.12	17.4 [215]
$C_7H_6N_2O_4$	327.5	2,6-dinitrotoluene 23.85 3*A10+A11+2*A12+2*A50+A1	0	72.82	50.7	23.85	16.6 [217]
$C_7H_6N_2O_4$	329.8	2,3-dinitrotoluene 17.57 3*A10+A11+2*A12+2*A50+A1	0	53.27	50.7	17.57	16.7 [217]
$C_7H_6N_2O_4$	329.5	3,4-dinitrotoluene 18.83 3*A10+A11+2*A12+2*A50+A1	0	57.15	50.7	18.83	16.7 [217]
$C_7H_6N_2O_5$	359.3	2-methyl-4,6-dinitrophenol 19.41 3*A12+A11+2*A10+A1+A31+2*A50	0	54.02	56.1	19.41	20.2 [215]
C_7H_6O	216	benzaldehyde 9.32 5*A10+A12+A34	0	43.1	51.1	9.32	11.0 [216]
$C_7H_6O_2$	395.5	benzoic acid 18.0 5*A10+A12+A36	0	45.45	43.0	18.0	17.0 [282]
$C_7H_6O_3$	431.8	2-hydroxybenzoic acid 24.6 4*A10+2*A12+A31+A36*B36	0	56.97	51.1	24.6	22.1 [216,8]
$C_7H_6O_3$	475.1	3-hydroxybenzoic acid 26.2 4*A10+2*A12+A31+A36*B36	0	55.15	51.1	26.2	24.3 [216,8]
$C_7H_6O_3$	488.1	4-hydroxybenzoic acid 30.9 4*A10+2*A12+A31+A36*B36	0	63.31	51.1	30.9	24.9 [233]
C_7H_7Br	271.8	benzylbromide 13.2 5*A10+A11+A2+A21	0	48.57	52.2	13.2	14.2 [49]
C_7H_7Br	301.2	4-bromotoluene 15.13 4*A10+A11+A12+A1+A21	0	50.2	47.1	15.1	14.3 [234]
C_7H_7Cl	280.7	*p*-chlorotoluene 13.55 A1+A12+A11+4*A10+A22	0	48.29	40.9	13.55	11.5 [234]
$C_7H_7ClN_2S$	413.5	1-(*o*-chlorophenyl)thiourea 22.29 4*A10+2*A12+A22*B22+A91	0	53.91	53.9	22.29	22.3 [221]
C_7H_7F	210.7	2-fluorotoluene 9.8 4*A10+A11+A12+A1+A24	0	46.51	46.8	9.8	9.9 [216]
C_7H_7F	184	3-fluorotoluene 8.3 4*A10+A11+A12+A1+A24	0	45.11	46.8	8.3	8.6 [216]
C_7H_7F	216.5	4-fluorotoluene 9.35 4*A10+A11+A1+A12+A24	0	43.18	46.8	9.35	10.13 [216]
C_7H_7I	299.5	benzyliodide 13.2 5*A10+A11+A2+A29	0	44.07	54.0	13.2	16.2 [46]
C_7H_7I	306.7	*p*-iodotoluene 14.96 4*A10+A11+A12+A29+A1	0	48.79	49.5	14.96	15.2 [234]
C_7H_7NO	402.3	benzamide 18.49 5*A10+A12+A61	0	45.96	57.5	18.49	23.1 [215]
$C_7H_7NO_2$	370	3-nitrotoluene 19.2 4*A10+A1+A11+A12+A50	0	51.88	47.9	19.2	17.7 [235]
$C_7H_7NO_2$		4-nitrotoluene					

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)
	318	16.9	53.1				
	324.8	16.81	0	51.76	47.9	16.81	15.6
		$4*A10+A12+A11+A1+A50$					[215]
$C_7H_7NO_2$		2-aminobenzoic acid					
	417.8	20.5	0	49.07	52.2	20.5	21.8
		$4*A10+2*A12+A36*B36+A45$					[215]
$C_7H_7NO_2$		3-aminobenzoic acid					
	452.9	21.84	0	48.12	52.2	21.84	23.6
		$4*A10+2*A12+A36*B36+A45$					[215]
$C_7H_7NO_2$		4-aminobenzoic acid					
	461.4	20.92	0	45.19	52.2	20.92	24.1
		$4*A10+2*A12+A36*B36+A45$					[215]
$C_7H_7NO_3$		4-nitro-5-methylphenol					
	401	27.4	0	68.33	53.3	27.4	21.4
		$3*A10+A1+A11+2*A12+A31+A50$					[215]
$C_7H_7NO_3$		2-nitro-5-methylphenol					
	302.8	20.79	0	68.66	53.3	20.79	16.1
		$3*A10+A1+A11+2*A12+A31+A50$					[215]
$C_7H_7N_3O_2$		N-acetyl-pyrazinamide					
	366.7	23.6	0	64.36	61.9	23.6	22.7
		$3*A10+A12+2*A41+A71+A1$					[9]
C_7H_8		toluene					
	178.0	6.62	0	37.15	45.0	6.62	8.0
		$5*A10+A1+A11$					[216]
C_7H_8		cycloheptatriene					
	154.0	2.35	15.24				
	198.0	1.16	5.86	21.11	38.5	3.51	7.6
		$A14+4*A15+6*A18$					[216]
C_7H_8		tetracyclo[3.2.0.0(2,7).0(4,6)]heptane					
	180	7.2	40				
	228	1.09	4.8	44.8	26.6	8.29	6.1
		$4*A14-5*A15+6*A16$					[216]
$C_7H_8N_2O$		phenylurea					
	420.6	23.68	0	56.3	52.1	23.68	21.9
		$5*A10+A12+A67$					[215]
$C_7H_8N_4O_2$		theophylline					
	544	28.2	0	51.84	44.6	28.2	24.3
	546.1	28.27	0	51.76	44.6	28.3	24.3
		$2*A14+3*A15+2*A125+A118+A121+2*A1+2*A19+A18*B18$					[236,205]
C_7H_8O		benzyl alcohol					
	257.6	8.79	0	34.11	36.4	8.79	9.4
		$5*A10+A11+A2+A30$					[215]
C_7H_8O		*o*-hydroxytoluene					
	304.2	15.82	0	52.01	50.4	15.82	15.3
		$A31+A1+A12+4*A10+A11$					[216]
C_7H_8O		*m*-hydroxytoluene					
	285.4	10.71	0	37.53	50.42	10.71	14.39
		$A31+A1+A12+4*A10+A11$					[216]
C_7H_8O		*p*-hydroxytoluene					
	307.9	12.72	0	41.25	50.42	12.72	15.52
		$A31+A1+A12+4*A10+A11$					[216]
C_7H_8O		methoxybenzene					
	268.7	12.9	0	48.0	51.9	12.9	13.9
		$5*A10+A12+A1+A32$					[216]
C_7H_8S		methylphenylsulfide					
	256.4	14.85	0	57.86	49.3	14.85	12.63
		$5*A10+A12+A1+A84$					[105]
$C_7H_9Cl_3NO_3PS$		O,O-dimethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate					
	318.7	25.92	0	81.32	73.2	25.92	23.3
		$4*A12+A10+A41+3*A22*E22+2*A1+A79$					[221]
$C_9H_{13}Cl_3NO_4P$		O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl)phosphate					
	312.5	15.61	0	49.97	76.4	15.61	23.9
		$4*A12+A10+A41+3*A22*E22+2*A1+A74+2*A2$					[221]
C_7H_9N		*m*-toluidine					
	241.7	8.8	0	36.41	51.5	8.8	12.5
		$A45+4*A10+A12+A1+A11$					[215]
C_7H_9N		*p*-toluidine					
	316.5	17.89	0	56.52	51.5	17.89	16.3
		$A45+4*A10+A12+A1+A11$					[215]

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_7H_9N		*o*-toluidine					
	249.6	8.08	0	32.37	51.5	8.08	12.9
		*A*45+4**A*10+*A*12+*A*1+*A*11					[215]
C_7H_9N		2-methylaniline					
	258	11.66	0	45.1	51.5	11.66	14.8
		4**A*10+*A*11+*A*12+*A*1+*A*45					[30]
C_7H_9N		2,3-dimethylpyridine					
	258.6	13.48	0	52.13	49.1	13.48	12.7
		2**A*1+2**A*11+3**A*10+*A*41					[69]
C_7H_9N		2,4-dimethylpyridine					
	209.4	8.82	0	42.12	49.1	8.82	10.3
		2**A*1+2**A*11+3**A*10+*A*41					[69]
C_7H_9N		2,5-dimethylpyridine					
	259.1	14.64	0	56.5	49.1	14.64	12.7
		2**A*1+2**A*11+3**A*10+*A*41					[69]
C_7H_9N		2,6-dimethylpyridine					
	267.1	13.04	0	48.82	49.1	13.04	13.1
		2**A*1+2**A*11+3**A*10+*A*41					[69]
C_7H_9N		3,4-dimethylpyridine					
	262.7	14.7	0	55.96	49.1	14.7	12.9
		2**A*1+2**A*11+3**A*10+*A*41					[69]
C_7H_9N		3,5-dimethylpyridine					
	266.9	13.11	0	49.12	49.1	13.11	13.1
		2**A*1+2**A*11+3**A*10+*A*41					[69]
$C_7H_9N_5O_{12}$		2,2,2-trinitroethyl 4,4-dinitropentanoate					
	363.8	20.08	55.2				
	366.7	6.69	18.26	73.46	89.6	26.78	32.9
		2**A*4**B*4+3**A*2+*A*1+5**A*50+*A*38					[122]
$C_7H_9N_5O_{12}$		2,2-dinitropropyl-4,4,4-trinitrobutyrate					
	284.2	25.94	91.28			-	
	335.5	20.92	62.35				
	368.2	6.69	18.18	171.8	89.6	53.56	33.0
		2**A*4**B*4+3**A*2+*A*1+5**A*50+*A*38					[122]
C_7H_{10}		bicyclo[2.2.1]hept-2-ene					
	130.3	4.27	32.77				
	319.5	3.48	10.89	43.66	37.8	7.75	12.1
		2**A*14+*A*15+2**A*16+2**A*18					[129,349]
$C_7H_{10}O$		2-norbornanone					
	368.7	3.39	0	9.19	39.7	3.39	14.6
		2**A*14+*A*15+2**A*16+*A*114					[217]
$C_7H_{10}N_2O$		6,7-diazatricyclo[3.2.2.0 2,4]non-6-ene-N-oxide					
	372.6	15.8	42.4				
	411.4	2.6	6.32	48.72	44.1	18.4	18.1
		3**A*14+2**A*16+2**A*16+*A*123					[42]
$C_7H_{10}N_2O_2$		N-acetyl-L-alanine amide					
	431	21.7	0	50.35	54.9	21.7	23.7
		2**A*1+*A*60+*A*3**B*3+*A*61					[278]
$C_7H_{10}N_2O_2$		1,3,6-trimethyluracil					
	384.5	21.2	0	55.14	38.4	21.2	14.8
		*A*14+3**A*15+2**A*125+3**A*1+*A*18**B*18+*A*19					[216]
$C_7H_{10}O_3$		3,3-dimethylpentanedioic anhydride					
	396.2	17.99	0	45.41	47.4	17.99	18.8
		*A*14+3**A*15+2**A*1+*A*17+*A*117					[237]
$C_7H_{11}N$		cyanocyclohexane					
	215	7.43	34.53				
	285.1	3.64	12.75	47.28	47.5	11.06	13.5
		*A*14+3**A*15+*A*16+*A*56					[216]
$C_7H_{11}N$		isocyanocyclohexane					
	192.6	6.18	32.07				
	279.6	4.23	15.12	47.19	47.2	10.4	13.2
		*A*14+3**A*15+*A*16+*A*57					[216]
C_7H_{12}		4-methylcyclohex-1-ene					
	153.6	6.63	0	43.16	44.1	6.63	6.77
		*A*14+3**A*15+*A*1+*A*16+2**A*18					[161]
C_7H_{12}		cycloheptene					
	154	5.28	34.29				
	210	0.71	3.38				
	217	0.97	4.47	42.14	45.0	6.96	9.8
		*A*14+4**A*15+2**A*18					[216,161]
$C_7H_{12}ClN_5$		6-chloro-N,N′-diethyl-1,3,5-triazine-2,4-diamine					
	502.5	47.35	0	94.23	65.3	47.35	32.8

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*A41+A22*F22+3*A12+2*A44+2*A1+2*A2					[221]
$C_7H_{12}O_2$		butyl acrylate					
	209.5	17.31	0	82.61	67.9	17.31	14.2
		A1+3*A2+A38+A5+A6*B6					[216]
$C_7H_{12}O_4$		pimilic acid					
	377.5	27.62	0	73.17	78.9	27.62	29.8
		5*A2*B2+2*A36*B36					[340]
$C_7H_{12}O_4S_2$		(*dl*) methylenebisthiopropionic acid					
	429	39.33	0	91.68	86.9	39.33	37.3
		2*A36*D36+2*A84+2*A3*B3+2*A1+A2					[273]
$C_7H_{12}O_4S_2$		(*d*) methylenebisthiopropionic acid					
	355	22.59	0	63.64	86.9	22.59	30.8
		2*A36*D36+2*A84+2*A3*B3+2*A1+A2					[273]
$C_7H_{13}N$		1-azabicyclo[2.2.2]octane					
	196	5.23	26.53				
	430	5.86	13.81	40.33	40.1	11.09	17.3
		2*A14+2*A15+A16+A119					[216]
$C_7H_{13}NO$		ζ-enantholactam					
	310.3	13.78	0	44.39	54.6	13.78	16.9
		A14+5*A15+A124					[216]
$C_7H_{13}N_3O_3S$		N,N-dimethyl-2-methylcarbamoyloxyimino-2-(methylthio)acetamide					
	372.2	30.17	0	81.04	59.4	30.17	22.1
		4*A1+A59+A7+A42+A69+A84					[221]
C_7H_{14}		cycloheptane					
	134.8	4.98	36.94				
	198.2	0.29	1.46				
	212.4	0.45	2.11				
	265.1	1.88	7.1	47.6	48.2	7.6	12.8
		4*A15+A14					[216]
C_7H_{14}		1,1-dimethylcyclopentane					
	146.8	6.49	44.18				
	203.7	1.09	5.34	49.52	41.4	7.57	8.4
		A14+A17+2*A1+2*A15					[216]
C_7H_{14}		*cis*-1,2-dimethylcyclopentane					
	141.5	6.65	47.01				
	219.4	1.66	7.55	54.57	46.5	8.31	10.2
		A14+2*A16+2*A1+2*A15					[216]
C_7H_{14}		*trans*-1,3-dimethylcyclopentane					
	139.5	7.4	0	53.09	46.5	7.4	6.5
		A14+2*A16+2*A1+2*A15					[216]
C_7H_{14}		ethylcyclopentane					
	134.7	6.87	0	51.0	50.8	6.87	6.8
		A14+A16+A1+A2+2*A15					[216]
C_7H_{14}		methylcyclohexane					
	146.6	6.75	0	46.1	47.3	6.75	6.9
		A14+A16+A1+3*A15					[216]
C_7H_{14}		1-heptene					
	154.3	12.66	0	82.5	77.5	12.66	12.0
		A1+4*A2*B2+A5+A6					[216]
$C_7H_{14}NO_5P$		dimethyl(E)-1-methyl-2-methylcarbamoylvinyl phosphate					
	326.9	22.36	0	68.4	55.0	22.36	18.0
		4*A1+A7+A6*B6+A60+A74					[221]
$C_7H_{14}N_2O_2S$		2-methyl-2(methylythio)propionaldehyde O-methylcarbamoyloxime					
	374.0	22.71	0	60.73	62.3	22.71	23.3
		4*A1+A4*B4+A6*B6+A69+A84+A42					[221]
$C_7H_{13}N_3O_3S$		N,N-dimethyl-2-methylcarbamoyloxyimino-2-(methylthio)acetamide					
	372.2	30.17	0	81.05	59.4	30.17	22.1
		4*A1+A59+A7+A84+A42+A69					[221]
$C_7H_{14}O$		heptanal					
	229.3	22.89	0	99.83	85.8	22.89	19.7
		A1+5*A2*B2+A34					[43]
$C_7H_{14}O$		diisopropyl ketone					
	204.8	11.2	0	54.6	55.3	11.2	11.3
		4*A1+2*A3*B3+A35					[216]
$C_7H_{14}O$		1-methylcyclohexanol					
	299.2	10.87	0	36.34	29.2	10.87	8.8
		A14+3*A15+A1+A17+A30					[230]
$C_7H_{14}O$		cycloheptanol					
	172.2	2.93	16.98				

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)	
	227.3	0.55	2.44					C_8H_5Cl
	258.4	0.88	3.39					
	280.3	1.6	5.72	28.53	35.2	5.96	9.9 [216]	$C_8H_5Cl_3$
		A14+4*A15+A30+A16						
$C_7H_{14}O_2$		heptanoic acid						
	224.8	2.04	9.08					
	265.8	15.44	58.07	67.15	77.6	17.48	20.6 [216,143]	$C_8H_5Cl_3$
		5*A2*B2+A1+A36						
$C_7H_{15}Cl_2N_2O_2P$		2-[*bis*(2-chloroethyl)amino]tetrahydro-2H-1,3,2-oxazophosphorine-2-oxide						
	322.6	33.13	0	102.7	102.7	33.13	33.1 [221]	C_8H_6
		A14+3*A15+A144+4*A2+2*A22*C22						
C_7H_{16}		heptane						
	182.6	14.04	0	76.9	81.8	14.04	14.9 [216]	$C_8H_6Cl_2$
		2*A1+5*A2*B2						
C_7H_{16}		2,4-dimethylpentane						
	154.0	6.85	0	44.46	44.7	6.85	6.9 [216]	$C_8H_6Cl_2$
		4*A1+A2+2*A3						
C_7H_{16}		3-ethylpentane						
	154.6	9.55	0	61.77	57.8	9.55	8.9 [216]	$C_8H_6Cl_2$
		3*A1+3*A2+A3						
C_7H_{16}		2-methylhexane						
	154.9	9.18	0	59.29	57.8	9.18	9.0 [216]	$C_8H_6Cl_2$
		3*A1+3*A2+A3						
C_7H_{16}		3,3-dimethylpentane						
	138.2	7.07	0	51.16	49.7	7.07	6.9 [216]	$C_8H_6Cl_4$
		4*A1+A4+2*A2						
C_7H_{16}		2,2,3-trimethylbutane						
	121	2.38	19.64					
	247.7	2.2	8.88	28.53	36.7	4.58	4.4 [216]	$C_8H_6Cl_4$
		5*A1+A3+A4						
C_7H_{16}		2,2-dimethylpentane						
	148.1	5.86	0	39.55	49.74	5.86	7.37 [215]	$C_8H_6Cl_4$
		4*A1+A4+2*A2						
$C_7H_{16}O$		1-heptanol						
	240.4	18.16	0	75.53	75.31	18.16	18.1 [216]	$C_8H_6N_2$
		A1+6*A2*B2+A30						
$C_7H_{16}O_2$		1,7-heptanediol						
	295.2	21.3	0	72.15	101.6	21.3	30.0 [215]	$C_8H_6N_2$
		7*A2*B2+2*A30*B30						
$C_7H_{16}S$		1-heptanethiol						
	229.9	25.4	0	110.4	96.6	25.4	22.2 [216]	$C_8H_6N_2$
		A1+6*A2*B2+A86						
$C_7H_{17}NSi$		N-(β-trimethylsilyethyl)ethylenimine						
	176.5	10.62	0	60.17	54.0	10.62	9.5 [216]	$C_8H_6N_2$
		3*A1+2*A2+A14+A119+A109						
$C_7H_{20}Si_2$		hexamethyldisilylmethane						
	140.7	11.11	0	78.98	58.5	11.11	8.2 [216]	$C_8H_6N_2$
		6*A1+2*A109+A2						
$C_8Cl_4N_2$		2,4,5,6-tetrachloro-1,3-benzenedicarbonitile						
	526.2	30	0	57.01	55.3	30	29.1 [221]	C_8H_6S
		4*A22*F22+2*A56+6*A12						
C_8F_{18}		perfluorooctane						
	176.5	3.14	17.79					
	254.2	9.58	37.69	55.48	93.8	12.72	23.8 [67]	C_8H_7Cl
		8*A4*B4+12*A26+6*A25						
$C_8H_3NO_5$		3-nitrophthalic anhydride						
	436.2	18.4	0	42.18	51.0	18.4	22.3 [179]	C_8H_7Cl
		A14+2*A15+A117+2*A19+A12+3*A10+A50						
$C_8H_3NO_5$		4-nitrophthalic anhydride						
	388.2	17.14	0	44.15	51.0	17.14	19.8 [179]	C_8H_7Cl
		A14+2*A15+A117+2*A19+A12+3*A10+A50						
$C_8H_4Cl_2O_2$		terephthalyl dichloride						
	337.3	2.34	6.92					
	356.1	21.1	59.25	66.18	66.2	23.44	23.6 [216]	C_8H_7Cl
		4*A10+2*A12+2*A40						
$C_8H_4N_2$		1,2-dicyanobenzene						
	414.1	20	0	48.3	50.2	20	20.8 [71]	C_8H_7Cl
		4*A10+2*A12+2*A56						
$C_8H_4O_3$		phthalic anhydride						
	403.3	23.09	0	57.25	48.2	23.09	19.4 [215]	C_8H_7F
		A14+2*A15+2*A19+A117+4*A10						

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)
$C_8H_5Cl_3O_2$		2,3,6-trichlorophenylacetic acid					
	432.3	22.43	0	51.89	68.5	22.43	29.6 [215]
		2*A10+3*A12+A11+A36*D36+3*A22*D22+A2					
$C_8H_5Cl_3O_3$		(2,4,5-trichlorophenoxy)acetic acid					
	431.2	38	0	88.13	75.3	38	32.5 [215]
		3*A22*E22+A32+A36*E36+4*A12+2*A10+A2					
$C_8H_5Cl_3O_4$		3,6-dichloro-5-hydroxy-2-methoxybenzoic acid					
	409.9	28.98	0	70.7	75.0	28.98	30.7 [215]
		2*A22*E22+A31+A32+A36*E36+5*A12+A10+A1					
C_8H_6		phenylacetylene					
	228	9.46	0	41.49	41.7	9.46	9.5 [132]
		5*A10+A12+A8+A9					
$C_8H_6Cl_2O_3$		(2,4-dichlorophenoxy)acetic acid					
	412.5	35.33	0	85.64	74.0	35.33	30.5 [221]
		3*A10+3*A12+A2+2*A22*D22+A36*D36+A32*D32					
$C_8H_6Cl_2O_3$		3,6-dichloro-2-methoxybenzoic acid					
	386.7	22.9	0	59.23	69.6	22.9	26.9 [215]
		4*A12+2*A10+2*A22*D22+A36*D36+A32*D32+A1					
$C_8H_6Cl_2O_3$		2,4-dichloro-2-methoxybenzoic acid					
	412.5	35.33	0	85.65	69.6	35.33	28.7 [215]
		4*A12+2*A10+2*A22*D22+A36*D36+A32*D32+A1					
$C_8H_6Cl_2O_4$		3,6-dichloro-5-hydroxy-2-methoxybenzoic acid					
	409.8	28.98	0	70.71	75.0	28.98	30.7 [215]
		A10+5*A12+2*A22*E22+A36*E36+A1+A32+A31					
$C_8H_6Cl_4$		tetrachloro-*o*-xylene					
	359.2	21.46	0	59.74	50.8	21.46	18.2 [215]
		4*A12+2*A11+2*A1+4*A22*D22					
$C_8H_6Cl_4$		tetrachloro-*p*-xylene					
	368.2	22.59	0	61.35	50.8	22.59	18.7 [215]
		4*A12+2*A11+2*A1+4*A22*D22					
$C_8H_6Cl_4O_4$		methyl tetrachloroterephthalic acid ester					
	444.3	16.89	0	38.03	92.7	16.89	41.2 [221]
		6*A12+2*A1+A38+4*A22*F22+A36					
$C_8H_6N_2$		phthalazine					
	364.5	13.32	0	36.54	51.4	13.32	18.7 [29]
		6*A10+2*A12+2*A41					
$C_8H_6N_2$		quinazoline					
	320.9	16.95	0	52.82	51.4	16.95	16.5 [29]
		6*A10+2*A12+2*A41					
$C_8H_6N_2$		quinoxaline					
	305.7	11.80	0	38.61	51.4	11.80	15.7 [29]
		6*A10+2*A12+2*A41					
$C_8H_6N_2OS_2$		6-methyl-1,3-dithiolo[4,5-*b*]quinoxalin-2-one					
	443.2	29.92	0	67.49	67.5	29.92	29.9 [221]
		A14+2*A15+A135+2*A19+2*A41+A1+A11 +3*A10+2*A12					
C_8H_6S		benzothiophene					
	304.5	11.82	0	38.82	44.1	11.82	13.4 [95]
		4*A10+A14+2*A15+A19+A18+A131+A19+A18*B18					
$C_8H_7ClO_3$		(*d*) *o*-chloromandelic acid					
	392.5	24.69	0	62.89	66.1	24.69	25.9 [220]
		4*A10+A11+A12+A3*B3+A30*C30+A36*C36+A22*C22					
$C_8H_7ClO_3$		(*dl*) *o*-chloromandelic acid					
	358.5	20.08	0	56.02	66.0	20.08	23.6 [220]
		4*A10+A11+A12+A3*B3+A30*C30+A36*C36+A22*C22					
$C_8H_7ClO_3$		(*dl*) *p*-chloromandelic acid					
	394	27.2	0	69.03	66.0	27.2	26.0 [220]
		4*A10+A12+A11+A3*B3+A30*C30+A36*C36+A22*C22					
$C_8H_7ClO_3$		(*d*) *p*-chloromandelic acid					
	394	23.01	0	58.41	66.0	23.01	26.0 [220]
		4*A10+A11+A12+A3*B3+A30*C30+A36*C36+A22*C22					
$C_8H_7Cl_2NO$		methyl-3,4-dichlorophenylcarbamate					
	381.4	23.19	0	60.8	60.4	23.19	23.0 [221]
		A1+3*A10+3*A12+2*A22*C22+A69					
$C_8H_7FO_3$		(*dl*) *m*-fluoromandelic acid					
	370	24.69	0	66.72	66.4	24.69	24.6

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)	
		4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24					[220,187]	
$C_8H_7FO_3$		(*d*) *m*-fluoromandelic acid						
	394	24.27	0	61.59	66.4	24.27	26.2	C
		4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24					[220,187]	
$C_8H_7FO_3$		(*dl*) *o*-fluoromandelic acid						
	390	30.12	0	77.24	66.4	30.12	25.9	C
		4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24					[220,187]	
$C_8H_7FO_3$		(*d*) *o*-fluoromandelic acid						
	363	20.92	0	57.63	66.4	20.92	24.17	C
		4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24					[220,187]	
$C_8H_7FO_3$		(*dl*) *p*-fluoromandelic acid						
	403	29.29	0	72.67	66.4	29.29	26.8	C
		4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24					[220,187]	
$C_8H_7FO_3$		(*d*) *p*-fluoromandelic acid						
	426	30.54	0	71.7	66.4	30.54	28.3	C
		4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24					[220,187]	
$C_8H_7ClO_3$		4-chlorophenoxyacetic acid						
	429.6	36.27	0	84.42	72.8	36.27	31.3	C
		4*A10+2*A12+A22*C22+A36*C36+A2+A32					[221]	
$C_8H_7N_3O_6$		2,4,6-trinitro-1,3-dimethylbenzene						
	455.4	38.49	0	84.52	54.1	38.49	24.64	C
		A10+2*A11+3*A12+2*A1+3*A50					[197]	
$C_8H_7N_5O_8$		2,4,6,N-tetranitro-N-methyltoluidene						
	375.6	19.33	0	51.46	54.3	19.33	20.4	C
		4*A12+A10+A11+3*A50+2*A1+A51+A49					[216]	
$C_8H_7N_5O_8$		2,4,6-N-tetranitroethylaniline						
	369	23.51	0	63.6	60.8	23.51	22.4	C
		A51+4*A12+2*A10+A1+A2+3*A50+A49					[216]	
C_8H_8		cubane						
	394	5.94	15.08					
	404.9	8.7	21.49	36.56	23.2	14.64	9.4	C
		5*A14−7*A15+8*A16					[150]	
C_8H_8		styrene						
	242.3	10.95	0	45.16	52.2	10.95	12.6	C
		5*A10+A5+A6+A12					[216]	
C_8H_8		cyclooctatetraene						
	268.5	11.27	0	41.49	39.0	11.27	10.5	C
		A14+5*A15+8*A18					[216]	
$C_8H_8BrCl_2O_3PS$		O-(4-bromo-2,5-dichlorophenyl)O,O-dimethyl phosphorothioate						
	325.3	31.15	0	95.74	71.1	31.15	23.1	C
		2*A10+4*A12+2*A1+2*A22*D22+A21+A79					[221]	
$C_8H_8Br_2$		α,α'-dibromo-*o*-xylene						
	368.2	26.78	0	72.73	59.8	26.78	22.0	C
		4*A10+2*A11+2*A2+2*A21*B21					[215]	
$C_8H_8Br_2$		α,α'-dibromo-*m*-xylene						
	350.2	23.69	0	67.65	59.8	23.69	21.0	C
		4*A10+2*A11+2*A2+2*A21*B21					[215]	
$C_8H_8ClNO_2$		N-methyl-2-chlorophenylcarbamic acid ester						
	362.7	21.81	0	60.12	59.1	21.81	21.4	C
		A1+4*A10+2*A12+A69+A22*B22					[221]	
$C_8H_8Cl_2$		α,α'-dichloro-*o*-xylene						
	328.2	21.26	0	64.78	57.1	21.26	18.7	C
		4*A10+2*A11+2*A2+2*A22*B22					[215]	
$C_8H_8Cl_2$		α,α'-dichloro-*m*-xylene						
	307.2	19.51	0	63.51	57.1	19.51	17.5	C
		4*A10+2*A11+2*A2+2*A22*B22					[215]	
$C_8H_8Cl_2$		α,α'-dichloro-*p*-xylene						
	373.2	23.97	0	64.23	57.1	23.97	21.3	C
		4*A10+2*A11+2*A2+2*A22*B22					[215]	
$C_8H_8Cl_2O_2$		1,4-dichloro-2,5-dimethoxybenzene						
	403.9	27.56	0	68.23	61.8	27.56	25.0	C
		4*A12+2*A10+2*A22*D22+2*A32*D32+2*A1					[215]	
$C_8H_8Cl_2O_3$		methyl 3,6-dichloro-2-methoxybenzoate						
	304.6	18.49	0	60.72	64.8	18.49	19.7	C
		2*A10+4*A12+2*A1+2*A22*D22+A38*D38+A32*D32					[221]	
$C_8H_8Cl_3O_3PS$		O,O-dimethyl O-(2,4,5-trichlorophenyl) phosphorothioate						

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)
	313.0	18.94	0	60.51	69.7	18.94	21.8
		2*A10+4*A12+3*A22*D22+2*A1+A79					[221]
$C_8H_8O_2$		*o*-toluic acid					
	376.9	20.17	0	53.51	43.5	20.17	16.4
		4*A10+A12+A11+A1+A36					[215]
$C_8H_8O_2$		*m*-toluic acid					
	381.9	15.73	0	41.19	43.5	15.73	16.6
		4*A10+A12+A11+A1+A36					[215]
$C_8H_8O_2$		*p*-toluic acid					
	452.8	22.72	0	50.17	43.5	22.72	19.7
		4*A10+A12+A11+A1+A36					[215]
$C_8H_8O_2$		phenylacetic acid					
	349.9	14.49	0	41.41	48.0	14.49	16.8
		5*A10+A11+A2+A36					[215]
$C_8H_8O_2$		methyl benzoate					
	261	13.9	0	53.26	54.8	13.9	14.3
		5*A10+A1+A38+A12					[247]
$C_8H_8O_2S$		phenyl vinyl sulfone					
	343.4	11.72	0	34.12	52.5	11.72	18.0
		5*A10+A5+A6+A12+A88					[238]
$C_8H_8O_3$		methyl 4-hydroxybenzoate					
	398.5	24.31	0	61	60.2	24.31	24.0
		4*A10+2*A12+A1+A31+A38*B38					[239]
$C_8H_8O_3$		(*dl*) mandelic acid					
	392	25.52	0	65.11	51.9	25.52	20.3
		5*A10+A3*B3+B30*A30+A36*B36+A11					[220]
$C_8H_8O_3$		(*d*) mandelic acid					
	406	23.36	0	64.92	51.9	26.36	21.1
		5*A10+A3*B3+B30*A30+A36*B36+A11					[220]
$C_8H_8O_3$		4-hydroxyphenylacetic acid					
	423.6	28.4	0	67.04	56.1	28.4	23.9
		4*A10+A11+A12+A2+A36*B36+A31					[215]
$C_8H_8O_3$		4-methoxybenzoic acid					
	457.8	28.4	0	62.04	53.1	28.4	24.3
	455.4	27.8	0	61.1	53.1	27.8	23.9
		4*A10+2*A12+A1+A36*B36+A32					[215,394]
$C_8H_9ClO_3$		(4-chloro-2-methylphenoxy)acetic acid					
	392.9	29.98	0	76.31	73.3	29.98	28.8
		3*A10+2*A12+A11+A22*C22+A36*C36+A32+A2+A1					[221]
C_8H_9NO		4-aminoacetophenone					
	379.2	38	0	100.2	58.2	38	22.1
		4*A10+2*A12+A35+A45+A1					[280]
C_8H_9NO		3-aminoacetophenone					
	371.2	29	0	78.12	58.2	29	21.6
		4*A10+2*A12+A35+A45+A1					[280]
C_8H_9NO		acetanilide					
	387.5	21.65	0	55.87	48.6	21.6	18.8
		5*A10+A12+A1+A60					[216]
$C_8H_9NO_2$		methyl 4-aminobenzoate					
	385.1	22.55	0	58.56	61.3	22.55	23.6
		4*A10+2*A12+A1+A45+A38					[239]
$C_8H_9NO_2$		*o*-hydroxyacetanilide					
	364.5	21.25	0	58.3	54.0	21.25	23.8
		4*A10+A60+A1+2*A12+A31					[216]
$C_8H_9NO_2$		*p*-hydroxyacetanilide					
	441.2	26.02	0	58.99	54.0	26.02	23.8
	441.7	27.0	0	60.9	54.0	27.0	23.8
		4*A10+A60+A1+2*A12+A31					[239,394]
$C_8H_9NO_2$		methyl N-phenylcarbamate					
	325	14.56	0	44.77	57.8	14.56	18.8
		5*A10+A12+A1+A69					[216]
$C_8H_9ClNO_5PS$		O-(2-chloro-4-nitrophenyl)O,O-dimethyl phosphorothioate					
	323.9	29.08	0	89.78	70.0	29.08	22.7
		2*A1+3*A10+3*A12+A22*C22+A50+A79					[221]
$C_8H_9O_3PS$		2-methoxy-4H-1,3,2-benzodioxaphosphorin 2-sulfide					
	327.86	16.92	0	51.61	51.6	16.92	16.9

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)
		$A14+3*A15+A19+A19+4*A10+A130+A1$					
C_8H_{10}		*o*-xylene					[221]
	247.8	13.6	0	54.9	45.6	13.6	11.3
		$2*A1+4*A10+2*A11$					
C_8H_{10}		*m*-xylene					[216]
	225.3	11.57	0	51.4	45.6	11.57	10.3
		$2*A1+4*A10+2*A11$					
C_8H_{10}		*p*-xylene					[216]
	286.3	17.11	0	59.77	45.6	17.11	13.1
		$2*A1+4*A10+2*A11$					
C_8H_{10}		ethylbenzene					[216]
	178.2	9.16	0	51.43	52.2	9.16	9.3
		$A1+A2+5*A10+A11$					
$C_8H_{10}N_4O_2$		caffeine					[216]
	426	0.94	2.21				
	512	23.43	45.76	47.97	40.7	24.37	20.9
	510.1	18.3	35.88	38.1	40.7	19.4	20.9
		$2*A14+3*A15+2*A125+3*A1+2*A19+A18*B18+A119+A118$					
$C_8H_{10}NO_5PS$		O,O-dimethyl O-4-nitrophenyl phosphorothioate					[227,395]
	308.2	20.07	0	65.12	68.7	20.07	21.2
		$4*A10+2*A12+2*A1+A50+A79$					
$C_8H_{10}O$		2,3-dimethylphenol					[215]
	346	21.02	0	60.75	51.0	21.02	17.6
		$3*A10+2*A11+A12+2*A1+A31$					
$C_8H_{10}O$		2,5-dimethylphenol					[215]
	348	23.38	0	67.18	51.0	23.38	17.7
		$3*A10+2*A11+A12+2*A1+A31$					
$C_8H_{10}O$		2,6-dimethylphenol					[215]
	318.9	18.9	0	59.27	51.0	18.9	16.3
		$3*A10+2*A11+A12+2*A1+A31$					
$C_8H_{10}O$		3,4-dimethylphenol					[215]
	334	18.13	0	54.28	51.0	18.13	17.0
		$3*A10+2*A11+A12+2*A1+A31$					
$C_8H_{10}O$		3,5-dimethylphenol					[215]
	336.8	18	0	53.44	51.0	18.0	17.2
		$3*A10+2*A11+A12+2*A1+A31$					
$C_8H_{10}O_2S$		benzylmethylsulfone					[215]
	400.5	25.52	0	63.73	52.5	25.52	21.0
		$5*A10+A11+A1+A2+A88$					
$C_8H_{11}N$		2,5-dimethylaniline					[276]
	279	13.7	0	49.1	52.1	13.7	14.5
		$3*A10+2*A11+A12+2*A1+A45$					
$C_8H_{11}N$		N,N-dimethylaniline					[51]
	275.6	11.56	0	46.28	42.5	11.56	11.7
		$5*A10+A12+A43+2*A1$					
$C_8H_{11}N$		exo-2-cyanobicyclo[2.2.1]heptane					[51]
	237.7	7.93	33.4				
	298.8	2.94	9.83	43.2	44.0	10.87	13.1
		$2*A14+A15+2*A16+A16+A56$					
$C_8H_{11}N$		endo-2-cyanobicyclo[2.2.1]heptane					[216]
	177.3	2.25	12.7				
	331.2	2.96	8.94	21.6	44.0	7.18	14.6
		$2*A14+A15+2*A16+A56+A16$					
$C_8H_{11}N$		2,4,6-trimethylpyridine					[216]
	229.0	9.54	0	41.64	50.0	9.54	11.4
		$3*A1+3*A11+2*A10+A41$					
$C_8H_{11}N_5$		6,8,9-trimethyladenine					[216]
	438	23.1	0	52.74	54.4	23.1	23.8
		$A14+2*A15+3*A19+3*A1+A118+A119+2*A41+A10+A12+A44$					
$C_8H_{11}N_5O_2$		2-amino-9-[(2-hydroxyethoxy)methyl]-9H-purine					[240]
	462.2	42.2	0	91.3	86.5	42.2	40.0
		$A14+2*A15+2*A19+A18*B18+2*A41+A45+A118+A119+3*A2+A30*F30+A32$					
$C_8H_{11}N_5O_3$		2-amino-9-[(2-hydroxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one					[203]
	528.2	30.44	0	57.63	92.7	30.44	48.9

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*A14+3*A15+3*A19+A18*B18+A124+2*A118+A45+A119+3*A2+A32+A30*F30					[203]
C_8H_{12}		2-bicyclo[2.2.2]octene					
	110.5	0.19	1.7				
	176.5	5.65	32				
	389.8	5.4	13.85	47.55	41.5	11.23	16.2
		2*A14+2*A15+2*A16+2*A18					[100]
C_8H_{12}		cycloocta-1,5-diene					
	194.4	−0.38					
	204	9.83	0	48.2	45.4	9.83	9.3
		A14+5*A15+4*A18					[216]
$C_8H_{12}NO_5PS_2$		O,O-dimethyl O-(4-aminosulfonylphenyl)phosphorodithioate					
	344.2	26.21	0	76.13	79.4	26.21	27.3
		2*A1+4*A10+2*A12+A96+A79					[221]
$C_8H_{12}N_2$		tetramethylsuccinonitrile					
	345	18.1	52.48				
	442	7.15	16.17	68.64	60.1	25.25	26.6
		4*A1+2*A4*B4+2*A56					[216]
$C_8H_{12}N_2O_2$		1,6-hexamethylene diisocyanate					
	206.1	18.64	0	90.46	102.2	18.64	21.1
		6*A2*B2+2*A58					[216]
$C_8H_{12}N_2O_3$		barbitol					
	462.6	24.98	0	54	63.1	24.98	29.2
		A14+3*A15+A128+A124+2*A1+2*A2+A17					[241]
$C_8H_{12}N_4O_{10}$		2,2-dinitropropyl 4,4-dinitropentanoate					
	330.6	23.01	69.61				
	370.8	6.28	16.93	86.53	89.4	29.29	33.2
		2*A4*B4+3*A2+2*A1+4*A50+A38					[122]
$C_8H_{12}N_4O_{10}$		2-methyl-2-nitropropyl 4,4,4-trinitrobutyrate					
	346.1	24.69	71.33				
	349.4	5.27	15.09	86.41	89.4	29.96	31.3
		2*A1+2*A4*B4+3*A2+4*A50+A38					[122]
$C_8H_{12}O_2$		1,4-cyclooctanedione					
	341.2	11.92	0	34.95	49.2	11.92	16.8
		A14+5*A15+2*A114					[114]
$C_8H_{13}ClN_2O_2$		5-chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1H,3H)-pyrimidinedione					
	448	12.51	0	27.92	64.6	12.51	28.9
		A14+3*A15+2*A19+A124+A125+4*A1+A4*B4+A22*C22					[221]
C_8H_{14}		*endo*-2-methylbicyclo[2.2.1]heptane					
	152.4	4.71	30.9				
	278.3	1.62	5.82	36.72	43.8	6.35	12.2
		2*A14+A15+A1+3*A16					[216]
C_8H_{14}		*exo*-2-methylbicyclo[2.2.1]heptane					
	164.1	8.38	0	51.0	43.8	8.38	7.2
		2*A14+A15+A1+3*A16					[216]
C_8H_{14}		bicyclo[2.2.2]octane					
	164.3	4.6	28.01				
	447.5	8.37	18.7	46.71	44.7	12.97	20.0
		2*A14+2*A16+2*A15					[215]
C_8H_{14}		cyclooctene					
	190.1	9.8	51.55				
	259.2	1.81	6.98	58.53	48.7	11.61	12.6
		A14+5*A15+2*A18					[161]
$C_8H_{14}N_4OS$		4-amino-6-(1,1-dimethylethyl)-3-(methylthio)1,2,4-triazin-5(4H)-one					
	399.4	18	0	45.06	58.2	18	23.3
		A14+3*A15+2*A19+4*A1+A4+A125+A84+A45+2*A118					[215]
$C_8H_{14}N_5Cl$		6-chloro-N-ethyl-N′-(isopropyl)-1,3,5-triazine-2,4-diamine					
	449.7	38.15	0	84.84	65.9	38.15	29.7
		3*A41+3*A12+2*A44+A22*F22+3*A1+A2+A3*B3					[221]
$C_8H_{14}N_6O_{10}$		1,7-diacetoxy-2,4,6-trinitro-2,4,6-triazaheptane					
	422.5	38.49	0	91.11	214.5	38.49	90.6
		2*A1+4*A2+2*A38+3*A51+3*A47					[216]
$C_8H_{14}O$		3-oxabicyclo[3.2.2]nonane					
	208.5	7.02	33.65				
	448.4	6.75	15.06	48.71	49.6	13.77	22.3
		2*A14+3*A15+2*A16+A112					[216]
$C_8H_{14}O_4$		suberic acid					
	415.3	28.82	0	69.4	88.2	28.82	36.6
		6*A2*B2+2*A36*B36					[340]

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)
$C_8H_{14}O_4$		tetramethylsuccinic acid					
	383	13.43	35.07				
	464	6.47	13.95	49.02	56.8	19.9	26.4 [216]
		4*A1+2*A4*B4+2*A36*B36					
$C_8H_{15}N$		3-azabicyclo[3.2.2]nonane					
	297.8	14.55	48.87				
	466.6	6.92	14.82	63.69	50.6	21.47	23.6 [216]
		2*A14+3*A15+2*A16+A121					
$C_8H_{15}NO_2$		dimethylaminoethyl methacrylate					
	237.7	16.85	0	70.9	59.1	16.85	14.0 [216]
		3*A1+2*A2+A5+A7+A38+A43					
C_8H_{16}		cyclooctane					
	166.5	6.32	37.94				
	183.8	0.48	2.6				
	288	2.41	8.35	48.89	51.9	9.2	14.9 [215]
		5*A15+A14					
C_8H_{16}		1,1-dimethylcyclohexane					
	153.2	5.98	39.05				
	239.8	2.01	8.37	47.43	45.1	7.99	10.8 [216]
		A14+A17+2*A1+3*A15					
C_8H_{16}		propylcyclopentane					
	155.8	10.04	0	64.45	57.9	10.04	9.0 [216]
		A14+A16+A1+2*A2+2*A15					
C_8H_{16}		*trans*-1,2-dimethylcyclohexane					
	185	10.5	0	56.77	50.2	10.5	9.3 [216]
		A14+3*A15+2*A1+2*A16					
C_8H_{16}		*cis*-1,2-dimethylcyclohexane					
	172.5	8.26	47.86				
	223.3	1.64	7.36	55.22	50.2	9.9	11.2 [216]
		A14+3*A15+2*A1+2*A16					
C_8H_{16}		*trans*-1,3-dimethylcyclohexane					
	183.1	9.87	0	53.93	50.2	9.87	9.2 [216]
		A14+3*A15+2*A1+2*A16					
C_8H_{16}		*cis*-1,3-dimethylcyclohexane					
	197.6	10.82	0	54.77	50.2	10.82	9.9 [216]
		A14+3*A15+2*A1+2*A16					
C_8H_{16}		*trans*-1,4-dimethylcyclohexane					
	236.2	12.34	0	52.26	50.2	12.34	11.9 [216]
		A14+3*A15+2*A1+2*A16					
C_8H_{16}		*cis*-1,4-dimethylcyclohexane					
	185.7	9.31	0	50.11	50.2	9.31	9.3 [216]
		A14+3*A15+2*A1+2*A16					
C_8H_{16}		ethylcyclohexane					
	161.4	8.28	0	51.3	54.5	8.28	8.8 [216]
		A14+A16+A1+A2+3*A15					
C_8H_{16}		1-octene					
	171.5	15.31	0	89.29	86.8	15.31	14.9 [216]
		A1+5*A2*B2+A5+A6					
C_8H_{16}		2,4,4-trimethyl-1-pentene					
	178.9	8.77	0	49.0	49.2	8.77	8.8 [216]
		4*A1+A2+A5+A7+A4					
C_8H_{16}		2,4,4-trimethyl-2-pentene					
	166	6.8	0	40.9	47.6	6.78	7.9 [216]
		5*A1+A4+A7+A6					
$C_8H_{16}N_2O_2$		N-acetyl-D-leucine amide					
	404	20.2	0	50	63.2	20.2	25.5 [216]
		3*A1+A3+A3*B3+A2+A61+A60					
$C_8H_{16}N_6$		1-(methylamino)-3,5-*bis*(dimethylamino)-*s*-triazine					
	378.8	22.34	0	58.98	48.4	22.34	18.3 [242]
		3*A41+3*A12+2*A43+A44+5*A1					
$C_8H_{16}N_6O$		1-(hydroxylamino)-3,5-*bis*(dimethylamino)-*s*-triazine					
	381.5	30.67	0	80.39	53.6	30.67	20.4 [242]
		4*A1+3*A41+3*A12+2*A43+A30*F30+A44					
$C_8H_{16}O$		octanal					
	288.2	25.86	0	89.73	95.1	25.86	27.4 [93]
		6*A2*B2+A1+A34					
$C_8H_{16}O$		2-octanone					
	252.86	24.42	0	96.57	86.4	24.42	21.8

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+5*A2*B2+A35					[216]
$C_8H_{16}O_2$		octanoic acid					
	289.7	21.35	0	73.8	86.9	21.35	25.2
		6*A2*B2+A1+A36					[216]
$C_8H_{16}O_2$		2,2,6,6-tetramethyl-1,3-dioxane					
	250.6	10.9	0	43.5	48.1	10.9	12.1
		A14+3*A15+2*A112+4*A1+2*A17					[47]
$C_8H_{16}O_2$		butyl butanoate					
	181.68	14.93	0	82.18	78.5	14.93	14.3
		2*A1+5*A2+A38					[216]
$C_8H_{16}O_2$		hexyl ethanoate					
	212.1	19.83	0	93.49	89.5	19.83	19.0
		2*A1+5*A2*B2+A38					[216]
C_8H_{18}		*n*-octane					
	216.38	20.74	0	95.86	91.1	20.74	19.7
		2*A1+6*A2*B2					[216]
C_8H_{18}		2,2,4-trimethylpentane					
	165.3	9.04	0	54.7	43.8	9.04	7.3
		5*A1+A4+A2+A3					[216]
C_8H_{18}		2,2,4-trimethylpentane					
	165.8	9.2	0	55.52	43.8	9.2	7.3
		5*A1+A2+A4+A3					[216]
C_8H_{18}		2,3,4-trimethylpentane					
	163.6	9.27	0	56.65	38.8	9.27	6.4
		5*A1+3*A3					[216]
C_8H_{18}		3-methylheptane					
	152.6	11.7	0	76.6	64.9	11.7	9.9
		3*A1+4*A2+A3					[216]
C_8H_{18}		2-methylheptane					
	164.2	11.92	0	72.62	64.9	11.92	10.7
		3*A1+4*A2+A3					[216]
C_8H_{18}		2,2,3,3-tetramethylbutane					
	152.5	2	13.11				
	373.9	7.54	20.16	33.28	35.8	9.54	13.4
		6*A1+2*A4					[216]
C_8H_{18}		4-methylheptane					
	152.2	10.84	0	71.22	64.9	10.84	9.9
		3*A1+A3+4*A2					[215]
$C_8H_{18}Cl_2Sn$		di-*n*-butyltindichloride					
	316.2	22.75	0	71.95	86.1	22.75	27.2
		2*A1+6*A2+2*A2*D22+A110					[130]
$C_8H_{18}N_2$		1,1-dimethylazoethane					
	242.6	4.89	20.16				
	258.6	10.28	39.75	59.91	56.3	15.17	14.6
		6*A1+2*A4*B4+2*A42					[42]
$C_8H_{18}N_2O$		1,1-dimethylazoxyethane					
	268	8.34	31.12				
	288.4	11.52	39.94	71.06	64.9	19.86	18.7
		6*A1+2*A4*B4+A54+A42					[42]
$C_8H_{18}N_2O_2$		*bis*-hydroxyethylpiperazine					
	405	25.9	0	63.95	80.2	25.9	32.5
		A14+3*A15+2*A119+4*A2+2*A30*D30					[216]
$C_8H_{18}N_4O_4$		N,N′-dimethyl-N,N′-dinitro-1,6-hexanediamine					
	331	61.68	0	186.35	113.0	61.68	37.4
		6*A2+2*A1+2*A43+2*A51					[225]
$C_8H_{18}O_2$		1,8-octanediol					
	332.8	36.1	0	108.47	111.0	36.1	36.9
		8*A2*B2+2*A30*B30					[215]
$C_8H_{18}O_4$		2,5,8,11-tetraoxadodecane					
	229.3	23.71	0	103.34	96.8	23.71	22.2
		2*A1+6*A2+4*A32					[216]
$C_8H_{18}S$		di-*n*-butyl sulfide					
	198.1	19.41	0	93.85	80.1	19.41	15.9
		2*A1+6*A2+A84					[216]
$C_8H_{18}S$		1-octanethiol					
	224	24.27	0	108.35	105.9	4.27	23.7
		A1+7*A2*B2+A86					[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)
$C_8H_{19}NSi$		N-(β-trimethylsilylethyl)trimethylenimine					
	199.4	12.9	0	64.68	57.7	12.9	11.5
		$A14+A15+A119+3*A1+2*A2+A109$					[216]
$C_8H_{20}Ge$		tetraethylgermane					
	180.3	12.31	0	68.29	63.7	12.31	11.5
		$4*A1+4*A2+A102$					[216]
$C_8H_{20}O_4Si$		tetraethoxysilane					
	187.7	13.2	70.32				
	191.0	11.14	58.33	128.66	90.6	24.34	17.3
		$4*A1+4*A2+4*A32+A109$					[10]
$C_8H_{20}Pb$		tetraethyllead					
	141.4	9.11	0	64.43	68.7	9.11	9.7
		$4*A1+4*A2+A106$					[216]
$C_8H_{20}Si$		tetraethylsilane					
	189.4	13.01	0	68.72	71.8	13.01	13.6
		$4*A1+4*A2+A109$					[227]
$C_8H_{20}Sn$		tetraethyltin					
	142.1	9.15	0	64.35	74.6	9.15	10.6
		$4*A1+4*A2+A110$					[216]
$C_8H_{24}O_4Si_4$		octamethylcyclotetrasiloxane					
	258	4.87	18.86				
	290.5	23.77	81.81	100.67	58.6	28.63	17.0
		$8*A1+A14+5*A15+4*A139+4*A112$					[216,98,121]
$C_8H_{28}N_4Si_4$		octamethylcyclotetrasilazane					
	367.7	25.05	0	68.13	62.5	25.05	23.0
		$8*A1+A14+5*A15+4*A139+4*A121$					[216]
$C_9H_4Cl_3NO_2S$		2-[(trichloromethyl)thiol]-1H-isoindole-1,3(2H)-dione					
	454.2	35.49	0	78.14	74.8	35.49	34.0
		$A14+2*A15+A128+2*A19+4*A10+A4*B4+A84+3*A22*E22$					[215]
$C_9H_4Cl_4O_4$		methyl tetrachloroterephthalic acid ester					
	444.3	16.89	0	38.01	75.1	16.89	33.4
		$4*A2*F22+A38+A36*F36+6*A12+A1$					[221]
$C_9H_4Cl_8O$		1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-isobenzofuran					
	395.4	25.94	0	65.61	47.4	25.94	18.7
		$3*A14+A15+3*A17+2*A19+4*A16+A112+8*A22*G22$					[232]
$C_9H_4O_5$		trimellitic anhydride 1,2,4-benzenetricarbozylic acid					
	385	10.46	0	27.18	33.3	10.46	12.8
		$A14+2*A15+3*A10+A12+A117+2*A19$					[216]
$C_9H_5N_4Cl_3$		4,6-dichloro-N-(2-chlorophenyl)-1,3,5-triazin-2-amine					
	431.0	31.48	0	73.04	68.2	31.48	29.4
		$4*A10+5*A12+3*A22*G22+3*A41+A44$					[221]
$C_9H_6Cl_2N_2O_3$		2-(3,4-dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione					
	396.3	29.5	0	74.42	63.6	29.5	25.2
		$A14+2*A15+A125+2*A22*E22+3*A10+3*A12+A1+A126$					[221]
$C_9H_6Cl_6O_4S$		6,7,8,9,10,10-hexachloro-6,9-methano-2,4,3-benzodioxathiapin-3,3-dioxide					
	419.7	21.66	0	51.6	51.6	21.66	21.7
		$3*A14+3*A15+6*A22*D22+3*A17+2*A19+A136+2*A16$					[221]
$C_9H_6O_2$		coumarin					
	342.1	19.14	0	55.95	48.0	19.14	16.4
		$A14+3*A15+A115+A18+A18+A19+A19+4*A10$					[82]
$C_9H_6O_2$		chromone					
	330.3	17.31	0	52.41	43.3	17.31	14.3
		$A14+3*A15+4*A10+A114+A112+2*A18*B18+2*A19$					[215,216]
$C_9H_7Cl_3O_3$		2-(2,4,5-trichlorophenoxy)propanoic acid					
	450.6	39.58	0	87.83	76.0	39.58	34.2
		$2*A10+4*A12+3*A22*E22+A36*E36+A32+A3*B3+A1$					[221]
$C_9H_7Cl_3O_3$		methyl 2-(2,4,5-trichlorophenoxy)acetate					
	361.9	30.46	0	84.18	70.5	30.46	25.5
		$2*A10+4*A12+A2+A32+A38+3*A22*E22+A1$					[221]
C_9H_7N		quinoline					
	220	0.07	0.31				
	258.4	10.66	41.27	41.58	47.9	10.73	12.4
		$7*A10+2*A12+A41$					[216]
C_9H_7N		isoquinoline					
	299.6	13.54	0	45.21	47.9	13.54	14.3
		$7*A10+2*A12+A41$					[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)
$C_9H_7N_3S$	460.2	5-methyl-1,2,4-triazolo[3,4-*b*]benzothiazole 24.07	0	52.3	49.1	24.07	22.6 [221]
		2*A14+2*A15+A1+3*A10+3*A19+A11+A119+2*A118+A131+A18*B18					
C_9H_8	271.7	indene 10.2	0	37.54	42.7	10.2	11.6 [216]
		4*A10+2*A15+A14+2*A18+2*A19					
$C_9H_8Cl_2O_3$	304.6	methyl 3,6-dichloro-2-methoxybenzoate 18.49	0	60.7	64.8	18.49	19.7 [215]
		4*A12+2*A10+2*A1+A38*D38+2*A22*D22+A32					
$C_9H_8Cl_2O_3$	389.2	2-(2,4-dichlorophenoxy)propanoic acid 30.43	0	78.18	74.8	30.43	29.1 [215]
		3*A10+3*A12+2*A22*D22+A36*D36+A32+A1+A3*B3					
$C_9H_8Cl_2O_3$	315.4	methyl 2,4-dichlorophenoxyacetate 25.1	0	79.59	69.3	25.1	21.8 [232]
		2*A22*D22+A1+3*A12+3*A10+A38+A32+A2					
$C_9H_8O_2$	406.2	cinnamic acid 22.63	0	55.71	52.1	22.63	21.2 [215]
		5*A10+A12+A6+A36+A6*B6					
$C_9H_8O_2$	341.2	allocinnamic acid 16.95	0	49.68	52.1	16.95	17.8 [215]
		5*A10+A12+A6+A36+A6*B6					
$C_9H_9BrO_3$	385	(*dl*) 2-(*p*-bromophenoxy)propanoic acid 31.8	0	82.59	74.9	31.8	28.8 [220]
		4*A10+2*A12+A1+A3*B3+A36*C36+A21+A32					
$C_9H_9BrO_3$	380	(*d*) 2-(*p*-bromophenoxy)propanoic acid 27.61	0	72.67	74.9	27.61	28.5 [220]
		4*A10+2*A12+A1+A3*B3+A36*C36+A21+A32					
$C_9H_9BrO_3$	349	(*dl*) 3-(*m*-bromophenyl)-3-hydroxypropanoic acid 26.78	0	76.73	74.6	26.78	26.1 [220]
		4*A10+A12+A11+C30*A30+A36*C36+A21+A2+A3*B3					
$C_9H_9BrO_3$	350	(*d*) 3-(*m*-bromophenyl)-3-hydroxypropanoic acid 23.85	0	68.14	74.6	23.9	26.1 [220]
		4*A10+A12+A11+C30*A30+A36*C36+A21+A3*B3+A2					
$C_9H_9BrO_3$	371	(*dl*) 3-(*p*-bromophenyl)-3-hydroxypropanoic acid 28.87	0	77.82	74.6	28.9	27.7 [220]
		4*A10+A12+A11+A21+C30*A30+A36*C36+A3*B3+A2					
$C_9H_9BrO_3$	398	(*d*) 3-(*p*-bromophenyl)-3-hydroxypropanoic acid 35.56	0	89.36	74.6	35.56	29.7 [220]
		4*A10+A12+A11+A21+C30*A30+A36*C36+A3*B3+A2					
$C_9H_9ClO_3$	388	(*dl*) 2-(*o*-chlorophenoxy)propanoic acid 32.22	0	83.03	73.4	32.22	28.5 [220]
		4*A10+2*A12+A1+A3*B3+A36*C36+A22*C22+A32					
$C_9H_9ClO_3$	369	(*d*) 2-(*o*-chlorophenoxy)propanoic acid 26.78	0	72.57	73.4	26.78	27.1 [220]
		4*A10+2*A12+A1+A3*B3+A36*C36+A22*C22+A32					
$C_9H_9ClO_3$	386	(*dl*) 2-(*m*-chlorophenoxy)propanoic acid 33.05	0	85.63	73.4	33.05	28.3 [220]
		4*A10+2*A12+A1+A3*B3+A36*C36+A22*C22+A32					
$C_9H_9ClO_3$	367.5	(*d*) 2-(*m*-chlorophenoxy)propanoic acid 29.71	0	80.83	73.4	29.71	27.0 [220]
		4*A10+2*A12+A1+A3*B3+A36*C36+A22*C22+A32					
$C_9H_9ClO_3$	357	(*dl*) 3-(*p*-chlorophenyl)-3-hydroxypropanoic acid 29.71	0	83.21	73.1	29.71	26.1 [220]
		4*A10+A12+A22*C22+C30*A30+A36*C36+A2+A3*B3+A11					
$C_9H_9ClO_3$	385	(*d*) 3-(*p*-chlorophenyl)-3-hydroxypropanoic acid 28.03	0	72.81	73.1	28.03	28.1 [220]
		4*A10+A12+A11+A22*C22+C30*A30+A36*C36+A3*B3+A2					
$C_9H_9ClO_3$	340	(*dl*) 3-(*m*-chlorophenyl)-3-hydroxypropanoic acid 23.85	0	70.14	73.1	23.85	24.9 [220]
		4*A10+A12+A11+A22*C22+C30*A30+A36*C36+A2+A3*B3					
$C_9H_9ClO_3$	368	(*d*) 3-(*m*-chlorophenyl)-3-hydroxypropanoic acid 28.03	0	76.18	73.1	28.03	26.9 [220]
		4*A10+A12+A11+A22*C22+C30*A30+A36*C36+A3*B3+A2					
$C_9H_9ClO_3$	392.9	(4-chloro-*o*-tolyloxy)acetic acid 29.98	0	76.3	73.3	29.98	28.8 [215]
		3*A10+2*A12+A11+A2+A1+A22*C22+A32+A36*C36					

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)
$C_9H_9Cl_2NO$		3′,4′-dichloropropionanilide					
	363.7	18.26	0	50.22	58.3	18.26	21.2
		$A1+A2+A60+3*A12+3*A10+2*A22*C22$					[215]
$C_9H_9FO_3$		(*dl*) 3-(*m*-fluorophenyl)-3-hydroxypropanoic acid					
	290	20.5	0	70.7	73.5	20.5	21.3
		$4*A10+A12+A11+A24+C30*A30+A36*C36+A2+A3*B3$					[220]
$C_9H_9FO_3$		(*d*) 3-(*m*-fluorophenyl)-3-hydroxypropanoic acid					
	311	24.27	0	78.03	73.5	24.27	22.9
		$4*A10+A12+A11+A24+C30*A30+A36*C36+A3*B3+A2$					[220]
$C_9H_9FO_3$		(*d*) 3-(*o*-fluorophenyl)-3-hydroxypropanoic acid					
	342	27.2	0	79.52	73.5	27.2	25.2
		$4*A10+A11+A12+A24+C30*A30+A36*C36+A2+A3*B3$					[220]
$C_9H_9FO_3$		(*d*) 3-(*o*-fluorophenyl)-3-hydroxypropanoic acid					
	348	22.59	0	64.92	73.5	22.59	25.6
		$4*A10+A11+A12+A24+C30*A30+A36*C36+A3*B3+A2$					[220]
$C_9H_9FO_3$		(*dl*) 3-(*p*-fluorophenyl)-3-hydroxypropanoic acid					
	362	27.61	0	76.28	73.5	27.61	26.6
		$4*A10+A11+A12+A24+C30*A30+A36*C36+A2+A3*B3$					[220]
$C_9H_9FO_3$		(*d*) 3-(*p*-fluorophenyl)-3-hydroxypropanoic acid					
	381	30.96	0	81.26	73.5	30.96	28.0
		$4*A10+A11+A12+A24+C30*A30+A36*C36+A3*B3+A2$					[220]
$C_9H_9NO_4$		[(benzoylamino)oxy] acetic acid					
	416.9	31.46	0	75.46	72.9	31.46	30.4
		$5*A10+A12+A60+A32+A2+A36*C36$					[215]
$C_9H_9NO_5$		(*dl*) 2-(*p*-nitrophenoxy)propanoic acid					
	411.4	32.22	0	78.31	74.9	32.22	30.8
		$4*A10+2*A12+A1+A3*B3+A36*C36+A32+A50$					[220]
$C_9H_9NO_5$		(*d*) 2-(*p*-nitrophenoxy)propanoic acid					
	362	20.92	0	57.79	74.9	20.92	27.1
		$4*A10+2*A12+A1+A3*B3+A36*C36+A32+A50$					[220]
C_9H_{10}		indane					
	221.8	8.6	0	38.77	45.9	8.6	10.2
		$4*A10+2*A19+A14+2*A15$					[216]
C_9H_{10}		α-methylstyrene					
	250.8	11.92	0	47.55	53.8	11.92	13.5
		$5*A10+A12+A1+A5+A7$					[216]
$C_9H_{10}Cl_2N_2O$		3-(3,4-dichlorophenyl)-1,1-dimethylurea					
	429.7	33.89	0	78.87	64.8	33.89	27.84
		$2*A1+2*A22*C22+3*A12+3*A10+A64*B64$					[232]
$C_9H_{10}BrClN_2O_2$		3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methylurea					
	369.8	26.54	0	71.79	68.7	26.54	25.4
		$2*A1+3*A10+3*A12+A32+A22*D22+A21+A64$					[221]
$C_9H_{10}Cl_2N_2O_2$		*N*′-(3,4-dichlorophenyl)-N-methoxy-N-methylurea					
	365.8	26.56	0	72.61	67.3	26.56	24.6
		$2*A22*D22+A32+A64+2*A1+3*A12+3*A10$					[215]
$C_9H_{10}O$		chroman					
	269.8	16.26	0	60.24	50.8	16.26	13.7
		$A14+3*A15+A19+A19+A112+4*A10$					[216]
$C_9H_{10}O$		isochroman					
	277.5	16.75	0	60.35	50.8	16.75	14.1
		$A14+3*A15+2*A19+A112+4*A10$					[216]
$C_9H_{10}O$		cinnamyl alcohol					
	308.2	15.73	0	51.04	49.0	15.73	15.1
		$5*A10+A12+2*A6+A2+A30$					[220]
$C_9H_{10}O$		4-ethylbenzoic acid					
	386.2	14.06	0	36.4	50.7	14.06	19.6
		$4*A10+A11+A12+A1+A2+A36$					[220]
$C_9H_{10}O_2$		hydrocinnamic acid					
	321.2	17.68	0	55.04	55.1	17.68	17.7
		$5*A10+A11+2*A2+A36$					[215]
$C_9H_{10}O_2$		phenyl glycidyl ether					
	279.8	17.32	0	61.9	61.3	17.32	17.2
		$A14+A112+A32*B32+16+A2+5*A10+A12$					[135]
$C_9H_{10}O_2S$		tolyl vinyl sulfone					
	340.4	10.88	0	31.96	53.0	10.88	18.0
		$4*A10+A11+A1+A5+A6+A88+A12$					[238]

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)
$C_9H_{10}O_3$	(*dl*) 3-phenyl-3-hydroxypropanoic acid					
366	29.71	0	81.17	59.2	29.71	21.7
	5*A10+A11+A2+A3*B3+B30*A30+A36*B36					[220]
$C_9H_{10}O_3$	(*d*) 3-phenyl-3-hydroxypropanoic acid					
391	32.64	0	83.47	59.2	32.64	23.1
	5*A10+A11+A2+A3*B3+A30*B30*+B36*A36					[220]
$C_9H_{10}O_3$	(*dl*) 2-phenoxypropionic acid					
388	33.05	0	85.19	58.2	33.05	22.6
	5*A10+A12+A1+A3*B3+A36*B36+A32*B32					[220]
$C_9H_{10}O_3$	(*d*) 2-phenoxypropionic acid					
359	22.59	0	62.93	58.2	22.59	20.9
	5*A10+A12+A1+A3*B3+A36*B36+A32*B32					[220]
$C_9H_{10}O_3$	4-methoxyphenylacetic acid					
358.1	21.8	0	60.88	58.1	21.8	20.8
	4*A10+A11+A12+A1+A2+A36*B36+A32*B32					[215]
$C_9H_{10}O_3$	4-hydroxyphenylpropionic acid					
402.5	28.9	0	71.8	63.2	28.9	25.5
	4*A10+A11+A12+2*A2+A36*B36+A31					[215]
$C_9H_{10}O_3$	4-ethoxybenzoic acid					
472.8	29.4	0	62.18	60.2	29.4	28.5
	4*A10+2*A12+A1+A2+A36*B36+A32*B32					[215]
$C_9H_{10}O_4$	(*dl*) erythro phenylglyceric acid					
395	31.38	0	79.44	71.9	31.38	28.4
	5*A10+A11+2*A3*B3+2*C30*A30+A36*C36					[220]
$C_9H_{10}O_4$	(*d*) erythro phenylglyceric acid					
371.5	23.43	0	63.07	71.9	23.43	26.7
	5*A10+A11+2*A3*B3+2*C30*A30+A36*C36					[220]
$C_9H_{11}BrN_2O$	N′-(4-bromophenyl)-N-methoxy-N-methyl urea					
368.3	24.44	0	66.36	67.4	24.44	24.8
	2*A1+A32*C32+4*A10+2*A12+A64*C64*+A21					[215]
$C_9H_{11}ClN_2O_2$	N′-(4-chlorophenyl)-N-methoxy-N-methyl urea					
353.4	22.54	0	63.78	66.0	22.54	23.3
	2*A1+4*A10+2*A12+A22*C22+A64*C64+A32					[215]
$C_9H_{11}ClN_2O$	3-(4-chlorophenyl)-1,1-dimethyl urea					
447.6	29.46	0	65.82	66.0	29.46	29.6
	2*A1+A64*B64+A22*B22+2*A12+4*A10					[215]
$C_9H_{11}ClO_3$	2-(4-chloro-2-methylphenoxy)propanoic acid					
366.2	26.43	0	72.16	73.9	26.43	27.1
	3*A10+2*A12+A11+A22*C22+A36*C36+A32*C32+A3*B3+2*A1					[221]
$C_9H_{11}Cl_3NO_3PS$	O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate					
315	24.53	0	77.86	87.5	24.53	27.6
	4*A12+A10+A41+3*A22*E22+2*A1+2*A2+A79					[215]
$C_9H_{11}N$	1,2,3,4-tetrahydroquinoline					
290	11.81	0	40.73	51.8	11.81	15.0
	A14+3*A15+A121+A19+4*A10+A19					[215]
$C_9H_{11}N$	5,6,7,8-tetrahydroquinoline					
222.7	9.08	0	40.75	53.1	9.08	11.8
	A14+3*A15+3*A10+A41+A19+A19					[215]
$C_9H_{11}NO_2$	ethyl phenyl carbamate					
326	16.27	0	49.79	64.9	16.27	21.2
	5*A10+A12+A1+A2+A69					[102]
$C_9H_{11}NO_2$	ethyl 4-aminobenzoate					
362.8	23.56	0	64.94	68.5	23.56	24.8
363.2	22.0	0	60.6	68.5	22.0	24.8
	4*A10+2*A12+A1+A2+A38+A5					[215,395]
$C_9H_{11}NO_2$	*p*-methoxyacetanilide					
400.3	27.82	0	69.51	56.0	27.82	22.4
	2*A1+4*A10+2*A12+A32+A60					[239]
C_9H_{12}	1,2,3-trimethylbenzene					
218.7	0.66	3				
230.3	1.33	5.8				
247.8	8.18	33.01	41.81	46.2	10.17	11.4
	3*A1+3*A10+3*A11					[216]
C_9H_{12}	1,2,4-trimethylbenzene					
229.3	13.19	0	57.53	46.2	13.19	10.59
	3*A1+3*A10+3*A11					[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_9H_{12}		1,3,5-trimethylbenzene						
	228.4	9.51	0	41.66	46.2	9.51	10.6	C_9H
		$3*A1+3*A10+3*A11$					[216,3]	
C_9H_{12}		isopropylbenzene						
	177.1	7.32	0	41.34	46.3	7.32	8.2	C_9H
		$2*A1+5*A10+A3+A11$					[92]	
C_9H_{12}		*n*-propylbenzene						
	173.6	9.27	0	53.39	59.3	9.27	10.3	C_9H
		$5*A10+A1+2*A2+A11$					[215]	
$C_9H_{12}ClN_5$		6-chloro-N-cyclopropyl-N′-(1-methylethyl)-1,3,5-triazine-2,4-diamine						
	441.6	28.76	0	65.13	60.0	28.76	26.5	C_9H
		$A14+A16+2*A1+A3*B3+A22*F22+3*A41+3*A12+2*A44$					[221]	
$C_9H_{12}N_2O$		1,1,-dimethyl-3-phenylurea						
	404.8	22.81	0	56.35	64.9	22.81	26.3	
		$2*A1+5*A10+A12+A64$					[215]	C_9H
$C_9H_{12}N_4O_2$		8-ethyltheophylline						
	545.3	37.2	0	68.22	60.2	37.2	32.8	
		$2*A14+3*A15+2*A125+A118+A121+3*A1+3*A19+A2$					[236]	
$C_9H_{13}BrN_2O_2$		5-bromo-6-methyl-3-(1-methylpropyl)-2,4(1H,3H)-pyrimidinedione						C_9H
	428.3	22.02	0	51.41	68.5	22.02	29.3	
		$A14+3*A15+A124+A125+3*A1+A2+A3*B3+A21+2*A19$					[215]	
$C_9H_{13}ClN_6$		2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2methylpropanenitrile						
	437.9	41.96	0	95.81	70.6	41.96	30.9	C_9H
		$3*A41+A22+2*A44+3*A1+A2+A4*B4+A56+3*A12$					[215]	
$C_9H_{13}N_5$		6,9-dimethyl-8-ethyladenine						
	436.8	29.8	0	68.22	61.5	29.8	26.9	C_9H
		$A14+2*A15+3*A19+3*A1+A118+A119+2*A41+A10+A12+A44+A2$					[240]	
$C_9H_{14}ClN_5$		2-chloro-4,6-bis(isopropylamino)-1,3,5-triazine						
	490.3	41.87	0	85.39	66.9	41.87	32.8	C_9H
		$A22*F22+2*A44+3*A41+3*A12+4*A1+2*A3*B3$					[215]	
$C_9H_{14}O_6$		glyceryl triacetate						
	275.3	25.8	0	93.73	80.2	25.8	22.1	
		$2*A2+3*A1+A3*B3+3*A38$					[216]	
$C_9H_{15}N_3O_8$		neopentyl-4,4,4-trinitrobutyrate						
	333.5	22.59	0	67.75	77.3	22.59	25.8	C_9H
		$3*A1+3*A2+A4+A4*B4+3*A50+A38$					[122]	
C_9H_{16}		*trans*-hexahydroindane						
	213.9	10.9	0	50.98	48.4	10.9	10.4	C_9H
		$2*A14+3*A15+2*A16$					[184]	
C_9H_{16}		*cis*-hexahydroindane						
	182.3	8.26	45.33					C_9H
	184.5	0.39	2.13					
	236.5	1.4	5.91	53.37	48.4	10.05	11.5	
		$2*A14+3*A15+2*A16$					[184]	
$C_9H_{16}ClN_5$		6-chloro-N-(1,1-dimethylethyl)-N′-ethyl-1,3,5-triazine-2,4-diamine						C_9H
	448.6	33.57	0	74.84	70.5	33.57	31.6	
		$4*A1+A2+A4*B4+2*A44+A22*F22+3*A41+3*A12$					[221]	
$C_9H_{16}N_4OS$		N-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-N,N′-dimethylurea						C_9H
	435.3	29.48	0	67.72	68.5	29.48	29.8	
		$5*A1+A4+A14+2*A15+A131+2*A118+2*A19+A64$					[215]	
$C_9H_{16}O_4$		azelaic acid						C_9H
	380	32.67	0	85.97	97.5	32.67	37.1	
		$2*A36*B36+7*A2*B2$					[215]	
$C_9H_{17}N$		*trans*-(R,S)-decahydroquinoline						C_9H
	321.4	25.72	0	80.02	54.3	25.72	17.5	
		$2*A14+4*A15+A16+A16+A121$					[215]	
C_9H_{18}		1-nonene						C_9H
	191.6	19.37	0	104.23	96.1	19.97	18.4	
		$A1+6*A2*B2+A5+A6$					[165]	
C_9H_{18}		*n*-butylcyclopentane						C_9H
	165.2	11.31	0	68.49	65.0	11.31	10.7	
		$A14+A16+3*A2+2*A15$					[216]	$C_{10}F$
C_9H_{18}		*n*-propylcyclohexane						
	178.3	10.37	0	58.19	61.6	10.37	11.0	
		$A14+A1+A16+2*A2+3*A15$					[215]	
$C_9H_{18}N_2O_2S$		3,3-dimethyl-1-(methylthio)-2-butanone O-methylcarbamoyloxime						
	330.2	19.83	0	60.04	60.4	19.83	20.0	$C_{10}F$