TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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*A14+A15+3*A16+A17+A27					[145]
$C_{10}H_{16}$		*d*-limonene					
	199.2	11.38		57.1	57.7	11.4	11.5
		2*A1+A5+A7+A16+A18+A19+A14+3*A15					[213,293]
$C_{10}H_{16}N_2O_2$		1,3-dimethyl-5-butyluracil					
	312.1	22.0		70.5	59.8	22.0	18.7
		A14+A15*3+2*A125+3*A1+3*A2+A18*B18+A19					[379]
$C_{10}H_{16}O$*		1-hydroxyadamantane					
	369.2	2.50	6.8		26.9	2.5	9.9
		3*A14+A15+3*A16+A17+A30					[172]
$C_{10}H_{16}O$*		2-hydroxyadamantane					
	325.2	0.30	0.92				
	391.2	3.74	9.56	10.5	32.1	4.0	12.6
		3*A14+A15+5*A16+A30					[172]
$C_{10}H_{18}O$*		cyclodecanone					
	294.9	24.3		82.3	57.9	24.3	17.1
		A14+7*A15+A114					[393]
$C_{10}H_{22}O$		1-decanol					
	280.1	37.66		134.5	103.0	37.7	28.9
		A1+9*A2*B2+A30					[321]
$C_{10}H_{23}AsO_2$*		dipentylarsinic					
	405	36.0		88.8	85.6	36.0	34.7
		2*A1+8*A2*B2+A142					[381]
$C_{10}H_{30}Si_5O_5$		decamethylcyclopentasiloxane					
	226.2	20.37		90.1	67.8	20.4	15.3
		10*A1+5*A112+5*A139+A14+7*A15					[121]
$C_{11}H_8N_2$		9H-pyrido[3,4-*b*]indole					
	471.5	25.50		54.0	56.5	25.5	26.6
		A14+2*A15+2*A19+2*A19+7*A10+A121+A41					[323]
$C_{11}H_{12}N_4O_2S$		sulfamerazine					
	515.2	31.6		61.2	79.4	40.9	31.6
		6*A10+3*A12+A11+A1+2*A41+A95+A45					[382]
$C_{11}H_{12}N_4O_3S$		4-amino-N-(6-methoxy-3-pyridazinyl)benzenesulfonamide (sulphamethoxypyridazine)					
	453.4	22.30		49.2	86.2	22.3	39.1
		6*A10+4*A12+A95+A45+2*A41+A1+A32					[194]
$C_{11}H_{12}N_2O$*		antipyrine					
	385.8	24.52		63.6	49.1	25.4	19.0
		A14+2*A15+2*A1+A119+A125+5*A10+A12+A19+A18*B18					[395]
$C_{11}H_{13}N_3O_3S$		sulfisoxazole					
	468.2	29.2		62.5	83.1	29.2	38.9
		4*A10+2*A12+A45+A95+A14+2*A15+3*A19+2*A1+A112+A118					[382]
$C_{11}H_{14}O_2$*		2-acetyl-3,5-dimethylanisole					
	323.2	0.99		3.06	63.4	1.0	20.4
		4*A1+2*A11+2*A12+2*A10+A32+A38					[11]
		Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent					
$C_{11}H_{14}O_3$*		4-*n*-butoxybenzoic acid					
	420.7	18.83	44.8				
	432.2	2.93	6.78	51.5	74.4	21.8	32.2
		4*A10+2*A12+3*A2+A1+A36*B36+A32					[178]
		Forms liquid crystal					
$C_{11}H_{16}O_2$*		1-adamantanecarboxylic acid					
	524.2	2.25		4.29	38.6	2.3	20.2
		3*A14+A15+3*A16+A17+A36					[149]
		Reported entropy is too small					
$C_{11}H_{20}O$*		cycloundecanone					
	287.7	23.0		80.5	61.6	23.0	17.7
		A14+8*A15+A114					[393]
$C_{11}H_{23}Br$		1-bromoundecane					
	263.3	33.47		127.1	128.1	33.5	33.7
		A1+10*A2*B2+A21					[333]
$C_{12}HF_{25}$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluorododecane					
	344.5	23.00		66.76	137.9	23.00	47.5
		11*A4*B4+3*A25+22*A26+A3*B3					[68]
$C_{12}H_8O_2S$		dibenzothiophene sulfone					
	507.8	23.72		46.7	40.4	23.7	20.5

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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)
		$A14+2*A15+2*A19+2*A19+8*A10+A134$					[327]
$C_{12}H_{10}N_2$		1-methyl-9H-pyrido[3,4-*b*]indole					
	509.9	27.20		53.3	57.1	27.2	29.1
		$A1+A14+2*A15+2*A9+2*A19+6*A10+A11+A121+A41$					[323]
$C_{12}H_{10}O_2$		α-naphthyl acetate					
	319.2	20.21		63.3	54.6	20.2	17.4
		$7*A10+3*A12+A1+A38$					[118]
$C_{12}H_{10}O_2$		β-naphthyl acetate					
	342.2	20.05		58.6	54.6	20.1	18.7
		$7*A10+3*A12+A1+A38$					[118]
$C_{12}H_{10}O_2S$		diphenyl sulfone					
	398.2	21.78		54.7	59.3	21.8	23.6
		$10*A10+2*12+A88$					[327]
$C_{12}H_{10}S$		diphenylsulfide					
	258.0	13.98		54.19	61.10	13.98	15.76
		$10*A10+2*A12+84$					[207]
$C_{12}H_{10}Te$*		diphenyl telluride					
	268.4	15.35		57.2	57.0	15.4	15.3
		$10*A10+2*A12+A140$					[300]
$C_{12}H_{12}N_2$		benzidine					
	400.2	19.10		47.7	72.0	19.1	28.8
		$4*A12+8*A10+2*A45$					[4]
$C_{12}H_{14}N_4O_2S$		4-amino-N-[2,6-dimethyl-4-pyrimidinyl)benzene sulfonamide					
	515.6	45.11		87.5	58.6	45.1	30.2
		$2*A1+5*A10+3*A12+2*A11+2*A41+A95$					[358]
$C_{12}H_{14}N_4O_2S$		sulfisomidine					
	523.6	42.7		81.5	80.0	42.7	41.9
		$5*A10+2*A41+A95+A45+3*A12+2*A11+2*A1$					[382]
$C_{12}H_{14}N_4O_2S$		sulfamethazine					
	471.6	31.1		66.0	80.0	31.1	37.7
		$5*A10+3*A12+2*A11+2*A1+2*A41+A95+A45$					[382]
$C_{12}H_{16}O_2$*		4-*n*-pentylbenzoic acid					
	252.0	2.60	10.32				
	362.0	9.90	27.35				
	395.0	1.50	3.80	41.47	57.7	14.0	22.8
	-	$A1+2*A2+4*A10+A11+A12+A36$					[177]
		Forms liquid crystal					
$C_{12}H_{16}O_3$*		4-*n*-pentoxybenzoic acid					
	398.2	21.8	54.7				
	422.2	2.1	5.0	59.7	81.5	23.9	34.4
		$4*A10+2*A12+4*A2+A1+A36*B36+A32$					[178]
		Forms liquid crystal					
$C_{12}H_{16}O_4$		2,5-dipropoxy-1,4-benzoquinone					
	357.0	8.60	24.09				
	460.8	33.6	72.92	97.0	84.0	42.2	38.7
		$2*A1+4*A2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114$					[342]
$C_{12}H_{16}O_6$		α-phenoxy-α-D-glucopyranoside					
	429.2	39.0		90.9	95.8	39.0	41.1
		$A14+3*A15+A2+A32+A112+4*A30*E30+5*A16+5*A10+A12$					[384]
$C_{12}H_{18}N_2O_3S$*		3-(*p*-tolyl-4-sulfonyl)-1-butyl urea					
	404.8	25.6		63.3		25.6	
		Group value not available					[358]
$C_{12}H_{18}O$		2-(1′-cyclohexenyl)cyclohexanone					
	278.8	17.26		61.9	59.0	17.3	16.5
		$2*A14+6*A15+A18+A19+A16+A114$					[314]
$C_{12}H_{18}O$		3,5-diisopropylphenol					
	326.3	12.13		37.2	53.4	12.1	17.4
		$4*A1+3*A10+2*A3+A31+2*A11+A12$					[330]
$C_{12}H_{18}O_6$		R,R,R-4,8,12-trimethyl-1,5,9-trioxacyclododeca-2,6,10-trione					
	380.2	21.5		56.6	84.7	21.5	32.2
		$3*A1+A14+9*A15+3*A115+3*A16$					[206]
$C_{12}H_{20}O$		2-cyclohexylcyclohexanone					
	277.0	18.00		65.0	58.2	18.0	16.1
		$2*A14+6*A15+2*A16+A114$					[314]
$C_{12}H_{22}O$		cyclododecanone					
	335.6	16.85		50.2	65.3	16.9	21.9
	336.3	16.6		50		16.6	
		$A14+A114+9*A15$					[298,393]
$C_{12}H_{22}O$		*trans*-2-cyclohexylcyclohexanol					

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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)
	325.8	14.52		44.6	46.6	14.5	15.2
		2*A14+6*A15+3*A16+A30					[313]
$C_{12}H_{31}AsO_2$*		dihexylarsinic acid					
	393	16.4	41.8				
	405	24.35	60.1	101.9	104.2	40.7	42.2
		2*A1+10*A2*B2+A142					[381]
$C_{12}H_{36}O_6Si_6$		dodecamethylcyclohexasiloxane					
	269.0	28.58		106.3	76.9	28.6	20.7
		12*A1+6*A112+6*A139+A14+9*A15					[121]
$C_{13}H_8O_2$		S-(+)-4-isobutyl-α-methylphenyl acetic acid					
	325.5	18.70		57.5	57.5	18.7	18.7
		3*A1+A2+A3+A3*B3+4*A10+2*A11+A36					[319]
$C_{13}H_{10}N_2O_2$*		N-phenyl 4-nitrobenzaldehyde imine					
	347.15	24.56		70.7	64.0	24.6	22.2
		9*A10+3*A12+A6*B6+A42+A50					[397]
$C_{13}H_{10}O_2$*		(2-hydroxyphenyl)phenylmethanone					
	308.2	0.67		2.17		0.67	
		No prediction made: Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent					[11]
$C_{13}H_{11}N$*		N-phenylbenzaldehyde imine					
	329.65	20.42		61.9	61.2	20.4	20.2
		10*A10+2*A12+A6*B6+A42					[397]
$C_{13}H_{12}N_2O$*		7-methoxy-1-methyl-9H-pyrido[3,4-*b*]indole					
	536.6	48.80		90.9	64.5	48.8	42.6
		2*A1+A14+2*A15+2*A19+2*A19+5*A10+A11+A121+A41+A32					[323]
$C_{13}H_{17}N_3O$*		aminopyrine					
	380	27.17		71.5	52.9	27.2	20.1
		A14+2*A15+4*A1+A43+A119+A125+5*A10+A12+2*A19					
$C_{13}H_{18}O_2$*		4-*n*-hexylbenzoic acid					
	371.0	17.40	46.90				
	380.0	2.40	6.31	53.21	65.1	19.80	24.7
		A1+2*A2+5*A10+A11+A12+A36					[177]
		Forms liquid crystal					
$C_{13}H_{18}O_2$		benzaldehyde 2,2-dimethylpropylene glycol acetal					
	307.6	18.6		60.5	60.2	18.6	18.5
		5*A10+A11+A14+3*A15+A17+A16+2*A1+2*A112					[385]
$C_{14}H_5F_{25}$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluorotetradecane					
	344.2	20.80		60.43	149.5	20.80	51.5
		12*A4*B4+3*A25+22*A26+A1+A2					[68]
		Amphiphillic compound					
$C_{14}H_9F_{17}O_2$*		perfluorooctylethylene methacrylate					
	210	5.0	23.8				
	253	9.0	35.6	59.4		14.0	
		Amphiphillic compound					[16]
$C_{14}H_9F_{21}O$*		ω-perfluorodecyl-1-butanol					
	360	21.30		59.2		21.3	
		Amphiphillic compound					[17]
$C_{14}H_{12}N_2O_2$		4-nitro-4′-methylbenzylidene aniline					
	402.0	27.30		67.9	64.6	27.3	25.9
		A1+8*A10+A11+3*A12+A42+A6*B6+A50					[302]
$C_{14}H_{12}O_2$*		(2-methoxyphenyl)phenylmethanone					
	350.2	0.68		1.94		0.7	
		No prediction made: Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent					[11]
$C_{14}H_{14}O_3$*		Naproxen					
	428.5	31.5		73.5	58.6	31.5	25.1
		2*A1+A3*B3+6*A10+A11+2*A12+A32+A36*B36					[394]
$C_{14}H_{20}O_4$		2,5-dibutoxy-1,4-benzoquinone					
	328.3	4.70	14.32				
	364.5	2.30	6.31				
	473.3	31.5	66.55	87.2	98.2	38.5	46.5
		2*A1+6*A2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114					[342]
$C_{14}H_{22}$		1,4-di-*tert*-butylbenzene					
	341.5	22.48		65.8	46.4	22.5	15.9
		6*A1+4*A10+2*A11+2*A4					[362]
$C_{14}H_{23}NO_2$		*n*-decyl-α-cyanoacrylate					
	294.5	41.80		142.0	133.3	41.8	39.3
		A1+9*A2*B2+A5+A7+A38+A56					[351]

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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)
$C_{14}H_{28}$		*trans*-1,4-di-*tert*-butylcyclohexane					
	363.2	17.15		47.2	51.1	17.2	18.6
		$6*A1+A14+2*A15+2*A4+2*A16$					[41]
$C_{14}H_{28}$		*cis*-1,4-di-*tert*-butylcyclohexane					
	293.2	8.79		30.0	51.1	8.8	15.0
		$6*A1+A14+2*A15+2*A4+2*A16$					[41]
$C_{14}H_{26}B_2N_4$*		4,4,8,8-tetraethylpyrazabole					
	342.4	28.61	83.61				
	379.2	3.22	8.49	92.1		31.8	
		Group value unavailable					[123]
$C_{14}H_{31}AsO_2$*		diheptylarsinic acid					
	299.0	30.1	100.7				
	389.0	20.3	52.3	153.0	122.8	50.4	47.7
		$2*A1+12*A2*B2+A142$					[381]
$C_{14}H_{42}O_7Si_7$		tetradecamethylcycloheptasiloxane					
	237.7	20.88		87.8	86.0	20.9	20.4
		$14*A1+7*A112+7*A139+A14+11*A15$					[121]
$C_{15}H_{11}NO_2$		1-(methylamino)-9,10-anthracenedione					
	443.2	28.81		65.0	49.1	28.8	21.8
		$A14+3*A15+2*A114+4*A19+7*A10+A1+A44+A12$					[315]
$C_{15}H_{12}ClN_5O_4$		5-[(4-chloro-2-nitrophenylazo]-1-ethyl-1,2-dihydro-6-hydroxy-4-methyl-2-oxo-3-pyridinecarbonitrile					
	500.2	35.16		70.3	85.8	35.2	42.9
		$3*A10+3*A12+A50+A22*F22+2*A42+A30*F30+2*A1+A2+A56+A14+3*A15+A125+4*A19$					[315]
$C_{15}H_{12}N_2O_2$		5,5-diphenylhydantoin					
	574.0	36.29		63.2	66.4	36.3	38.1
		$A14+2*A15+2*A124+A17+10*A10+2*A11$					[395]
$C_{15}H_{14}O_2$*		(2-hydroxy-4,6-dimethylphenyl)phenylmethanone					
	405.2	0.67		1.65		0.67	
		No prediction made: Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent					[11]
$C_{15}H_{16}S_2$		2,2-bis(phenylthio)propane					
	329.0	24.4		74.2	75.4	24.4	24.8
		$2*A1+10*A10+2*A12+A4*B4+2*A84$					[363]
$C_{15}H_{20}N_2O_4S$*		4-acetyl-N-[(cyclohexylamino)carbonyl]benzene sulfonamide					
	457.0	41.08		89.9		41.1	
		Group value not available					[358]
$C_{15}H_{21}NO_2$		1-methyl-4-phenylpiperidine-4-carboxylic acid ethyl ester (meperidine)					
	308.2	24.60		79.8	68.0	24.6	21.0
		$2*A1+5*A10+A11+A38+A14+3*A15+A2+A17+A119$					[296]
$C_{16}H_9F_{25}$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosafluorohexadecane					
	147	0.70	4.76				
	314	1.40	4.46				
	349	21.0	60.17	69.39	163.7	23.1	57.2
		$3*A2+A1+12*A4*B4+3*A25+22*A26$					[17]
$C_{16}H_{14}O_3$		Amphiphillic compound (±)α-(3-benzoylphenyl)propionic acid					
	367.4	28.23		76.8	70.6	28.2	25.9
		$9*A10+A11+2*A12+A35+A36*B36+A1+A3*B3$					[209]
$C_{16}H_{16}$		2,2-metacyclophane					
	404.0	21.42		53.0	51.3	21.4	20.7
		$A14+7*A15+4*A19+2*A18+6*A10$					[316]
$C_{16}H_{16}$		2,2-metaparacyclophane					
	315.0	0.98	3.11				
	354.0	12.76	36.05	39.2	46.0	13.7	16.3
		$A14+8*A15+4*A19+3A18+5*A10$					[316]
$C_{16}H_{16}$*		2,2-paracyclophane					
	323.2	0.21		0.65	40.7	0.2	13.2
		$A14+9*A15+4*A19+4*A18+4*A10$					[360]
$C_{16}H_{16}O_2$*		(2-hydroxyphenyl)-2,4,6-trimethylphenylmethanone					
	353.2	0.49		1.39		0.49	
		No prediction made. Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent					[11]
$C_{16}H_{17}ClN_4O_4$*		2,2′-[[3-chloro-4-[(4-nitrophenyl)azo]phenyl]imino]bis-ethanol					
	463.2	29.78		64.3		29.8	
		Group value not available					[13]

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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)
$C_{16}H_{17}Cl_2N_5O_4$*		1-[[2-chloro-4-[(2-chloro-4-nitrophenyl)azo]-5-(methylamino)phenyl]amino]-2-propanol N-oxide					
	371.2	30.62		82.5	82.5	30.6	30.6
		Group value not available					[315]
$C_{16}H_{17}F_{15}O$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7-pentadecafluoro-8-hexadecanone					
	285.8	34.20		119.7	147.5	34.2	42.2
		$7*A4*B4+3*A25+12*A26+A1+7*A2+A35$					[23]
		Amphiphillic compound					
$C_{16}H_{20}O_3$		3-benzoyl-1,2,2-trimethylcyclopentanecarboxylic acid					
	387.6	20.35		52.5	60.0	20.4	23.3
		$3*A1+A14+2*A15+2*A17+A16+2*A10+A12+A36*B36+A35$					[366]
$C_{16}H_{23}N$*		N-cyclohexyl(2,4,6-trimethyl)benzaldehyde imine					
	339.4	25.61		75.5	92.1	25.6	31.2
		$A14+3*A15+A16+3*A1+2*A10+A6*B6+A42+A12$					[397]
$C_{16}H_{24}O_4$		2,5-dipentoxy-1,4-benzoquinone					
	333.7	9.0	26.97				
	414.6	36.5	88.04	115.0	112.5	45.5	46.6
		$2*A1+8*A2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114$					[342]
$C_{16}H_{35}AsO_2$*		dioctylarsinic acid					
	379	20.7	54.6				
	402	35.8	89	143.6	141.4	56.5	56.6
		$2*A1+14*A2*B2+A142$					[381]
$C_{17}H_{16}ClN_5O_3$		3-[[4-[(2-chloro-4-nitrophenyl)azo]phenyl](2-hydroxyethyl)amino]propanenitrile					
	428.2	26.29		61.4	90.7	26.3	38.8
		$4*A2+7*A10+5*A12+A30*F30+A22*F22+A50+A56+2*A42+A43$					[315]
$C_{17}H_{17}ClO_6$*		([2S]-*trans*-7-chloro-,2′,4,6-trimethoxy-6′-methylspiro[benzofuran-2(3H),1′-(2)cyclohexene]-3,4′-dione					
	495.2	39.39		79.6	77.8	39.4	38.5
		$4*A1+A10+3*A12+2*A14+4*A15+A112+2*A114+3*A32+A22*F22+A17+A18+3*A19+A16$					[357]
$C_{17}H_{17}Cl_2N_5O_4$		N-[4-chloro-2-[(2-chloro-4-nitrophenyl)azo]-5-[(2-hydroxypropyl)amino]phenyl] acetamide					
	471.2	38.87		82.5	81.9	38.9	38.6
		$5*A10+7*A12+2*A22*F22+2*A1+A2+A3*B3+A30*F30+A50+2*A42+A60+A44$					[315]
$C_{17}H_{19}NO_3$		7,8-didehydro-4-5-epoxy-17-methylmorphinan-3,6-diol (morphine)					
	528.2	28.87		54.7	73.9	28.9	39.0
		$4*A14+3*A15+3*A16+A17+A119+A1+2*A18+A30*D30+3*A19+2*A10+A12+A112+A31+A114$					[296]
$C_{17}H_{19}NO_3$		4,5-epoxy-3-hydroxy-17-methylmorphinan-6-one (hydromorphone)					
	539.2	35.61		66.0	54.8	35.6	29.5
		$2*A10+4*A14+3*A15+3*A19+A31+A112+A1+A119+3*A16+A12+A17+A114$					[296]
$C_{17}H_{21}ClO_4$		3-(3-chloro-4-methoxybenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
	440.2	29.10		66.1	82.7	29.1	36.4
		$4*A1+A14+2*A15+2*A17+A16+3*A10+3*A12+A36*D36+A35+A32+A22*D22$					[366]
$C_{17}H_{21}F_{15}$*		1,1,1,2,3,3,4,4,5,5,6,6-dodecafluoro-2-(trifluoromethyl)hexadecane					
	220.0	3.00	13.64				
	261.0	18.00	68.96	82.6	143.8	21.0	37.5
		$7*A4*B4+6*A25+A27+8*A26+A1+9*A2$					[22]
		Amphiphillic compound					
$C_{17}H_{21}NO_6$		3-(3-nitro-4-methoxybenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
	426.9	32.36		75.8	84.2	32.4	35.9
		$4*A1+A14+2*A15+2*A17+A16+3*A10+3*A12+A36*D36+A35+A32+A50$					[366]
$C_{17}H_{21}N_3O_2$		2,2′-[[3-methyl-4-4(phenylazo)phenyl]imino]bis-ethanol					
	384.2	31.90		83.0	88.4	31.9	34.0
		$8*A10+3*A12+A11+2*A42+A1+4*A2+2*A30*E30+A43$					[13]
$C_{17}H_{22}O_3$		3-(4-methylbenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
	468.2	30.07		64.2	60.6	30.1	28.4
		$4*A1+A14+2*A15+2*A17+A16+4*A10+A11+A12+A36*B36+A35$					[372]
$C_{17}H_{23}NO_3$*		3-[(hydroxyimino)phenylmethyl]-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester					
	422.0	33.80		80.1	67.4	33.8	28.4
		$4*A1+A14+2*A15+A12+5*A10+2*A17+A7+A53+A38+A16$					[373]
$C_{17}H_{23}NO_4$*		3-(4-methoxy-3-aminobenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
	498.6	41.32		82.9	87.9	41.3	43.8
		$4*A1+A14+2*A15+2*A17+A16+3*A10+3*A12+A36*D36+A35+A32+A45$					[366]

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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)
$C_{18}HF_{15}Ge$*	tris(pentafluorophenyl)germane					
405.0	34.90		86.2	86.2	34.9	34.9
	18*A12+15*A24+A141					[308]
$C_{18}H_{11}NO_3$	2-(3-hydroxy-2-quinolinyl)-1H-indene-1,3(2H)-dione					
539.2	30.89		57.3	80.3	30.9	43.3
	9*A10+4*A12+A14+2*A15+4*A19+A114+A30*D30+A41					[315]
$C_{18}H_{13}F_{25}$*	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluorooctadecane					
317.2	3.30	10.4				
352.2	21.80	61.70	72.10	177.9	25.10	62.7
	12*A4*B4+3*A25+22*A26+A1+5*A2					[68]
	Amphiphillic compound					
$C_{18}H_{20}$	6-(4-biphenyl)-1-hexene					
274.5	15.10		55.0	93.0	15.1	25.5
	9*A10+2*A12+A11+4*A2+A5+A6					[97]
$C_{18}H_{20}$	3,3-paracyclophane					
332.0	7.36	22.17				
351.0	0.46	1.31				
377.0	11.76	31.19	54.7	48.1	19.6	18.1
	A14+11*A15+4*A19+4*A18+4*A10					[316]
$C_{18}H_{20}O_2$*	(2-hydroxyl-4,6-dimethylphenyl)-2,4,6-trimethylphenylmethanone					
380.2	0.84		2.21		0.84	
	Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent					[11]
$C_{18}H_{21}N$*	N-benzyl-pivalophenone imine					
339.6	27.86		82.05	84.2	27.9	28.6
	10*A10+A11+A12+3*A1+A4+A2+A6*B6+A42					[397]
$C_{18}H_{21}NO_3$	7,8-didehydro-4,-5-epoxy-3-methoxy-17-ethylmorphanan-6-ol (codeine)					
430.3	23.81		55.3	62.6	23.8	38.5
	2*A10+4*A14+3*A15+3*A19+A112+2*A1+A119+4*A16+A12+A17+A32+A30*D30+2*A18					[374]
$C_{18}H_{22}O_4$	4,4′-di-(2-methoxyethoxy)biphenyl					
409.5	17.53	42.81				
412.4	22.67	54.97	97.8	111.6	40.2	40.3
	2*A1+4*A2+8*A10+4*A12+4*A32					[345]
$C_{18}H_{24}N_2O_6$*	3-[(hydroxyimino)(4-methoxy-3-nitrophenyl)methyl]-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester					
433.0	31.99		73.9	77.6	32.0	33.6
	5*A1+A14+2*A15+3*A12+3*A10+2*A17+A16+A38+A32 +A50+A7+A53					[373]
$C_{18}H_{24}O_3$	3-(4-ethylbenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
387.6	22.54		58.2	67.7	22.5	26.3
	4*A1+A14+2*A15+2*A17+A16+4*A10+A2+A11+A12+A36*B36+A35					[366]
$C_{18}H_{24}O_3$	3-(3,4-dimethylbenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
460.6	32.31		70.2	61.2	32.3	28.2
	5*A1+A14+2*A15+2*A17+A16+3*A10+2*A11+A12+A36*B36+A35					[366]
$C_{18}H_{24}O_3$	3-(2,4-dimethylbenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
386.8	18.81		48.6	61.2	18.8	23.7
	5*A1+A14+2*A15+2*A17+A16+3*A10+2*A11+A12+A36*B36+A35					[366]
$C_{18}H_{24}O_4$	3-(4-ethoxybenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
394.6	22.05		55.9	88.5	22.1	34.9
	4*A1+A14+2*A15+2*A17+A16+4*A10+A2+2*A12+A36*C36+A35+A32					[366]
$C_{18}H_{25}NO_3$	3-[4-(dimethylamino)benzoyl]-1,2,2-trimethylcyclopentanecarboxylic acid					
445.0	25.03		56.3	72.1	25.0	32.1
	5*A1+A14+2*A15+2*A17+A16+4*A10+2*A12+A36*C36+A35+A43					[366]
$C_{18}H_{25}NO_4$*	3-[(hydroxyimino)(4-methoxyphenyl)methyl]-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester					
433.0	36.99		85.4	74.8	37.0	32.4
	5*A1+A14+2*A15+2*A12+4*A10+2*A17+A16+A38+A32+A53+A7					[373]
$C_{18}H_{28}O_4$	2,5-di-*n*-hexyloxy-1,4-benzoquinone					
332.3	5.3	15.95				
412.1	38.9	94.39	110.3	126.6	44.2	52.2
	2*A1+10*A2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114					[342]
$C_{18}H_{32}O_2$	linoelaidic acid					
303	47.70		157.4	163.8	47.7	49.6
	A1+12*A2*B2+4*A6+A36					[331]
$C_{18}H_{32}O_2$	4-octadecynoic acid					

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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)	
	348	57.94		166.5	151.2	57.9	52.6	C
		A1+12*A2*B2+2*A9+A36+2*A2					[331]	
$C_{18}H_{32}O_2$		5-octadecynoic acid						
	325	54.41		167.4	149.0	54.4	48.4	C
		A1+11*A2*B2+2*A9+A36+3*A2					[331]	
$C_{18}H_{32}O_2$		6-octadecynoic acid						
	324	54.92		169.5	155.6	54.9	50.4	C
		A1+14*A2*B2+2*A9+A36					[331]	
$C_{18}H_{32}O_2$		7-octadecynoic acid						
	322	53.61		166.5	155.6	53.6	50.1	C
		A1+14*A2*B2+2*A9+A36					[331]	
$C_{18}H_{32}O_2$		8-octadecynoic acid						
	320	55.30		172.8	155.6	55.3	49.8	C
		A1+14*A2*B2+2*A9+A36					[331]	
$C_{18}H_{32}O_2$		9-octadecynoic acid						
	319	54.87		172.0	155.6	54.9	49.6	C
		A1+14*A2*B2+2*A9+A36					[331]	
$C_{18}H_{32}O_2$		10-octadecynoic acid						
	319	52.23		164.0	155.6	52.3	49.6	C
		A1+14*A2*B2+2*A9+A36					[331]	
$C_{18}H_{32}O_2$		11-octadecynoic acid						
	320	55.97		174.9	155.6	56.0	49.8	
		A1+14*A2*B2+2*A9+A36					[331]	
$C_{18}H_{32}O_2$		12-octadecynoic acid						C
	320	49.79		155.6	155.6	49.8	49.8	
		A1+14*A2*B2+2*A9+A36					[331]	
$C_{18}H_{32}O_2$		13-octadecynoic acid						C
	322	55.51		172.4	155.6	55.5	50.1	
		A1+14*A2*B2+2*A9+A36					[331]	
$C_{18}H_{32}O_2$		14-octadecynoic acid						
	337	52.74		156.5	151.2	52.7	51.0	C
		A1+12*A2*B2+2*A9+A36+2*A2					[331]	
$C_{18}H_{32}O_2$		16-octadecynoic acid						
	347	60.10		173.2	155.6	60.1	54.0	C
		A1+14*A2*B2+2*A9+A36					[331]	
$C_{18}H_{32}O_2$		17-octadecynoic acid						
	340	54.20		159.4	157.7	54.2	52.9	C
		15*A2*B2+A9+A36+A8					[331]	
$C_{18}H_{34}B_4N_4$*		4,4,8,8-tetrapropylpyrazabole						
	382.2	33.00		86.3		33.0		C
		Group value unavailable					[123]	
$C_{18}H_{34}O_2$		*trans*-3-octadecenoic acid						
	334	57.15		171.1	169.6	57.2	56.7	C
		A1+13*A2*B2+2*A6+A36+A2					[331]	
$C_{18}H_{34}O_2$		*trans*-4-octadecenoic acid						
	333	55.88		167.8	167.4	55.9	55.7	
		A1+12*A2*B2+2*A6+A36+2*A2					[331]	
$C_{18}H_{34}O_2$		*trans*-5-octadecenoic acid						C
	319	45.11		141.3	165.2	45.1	52.7	
		A1+11*A2*B2+2*A6+A36+3*A2					[331]	
$C_{18}H_{34}O_2$		*trans*-6-octadecenoic acid						C
	326	60.15		184.5	171.8	60.2	56.0	
		A1+14*A2*B2+2*A6+A36					[331]	
$C_{18}H_{34}O_2$		*trans*-10-octadecenoic acid						
	326	58.52		179.5	171.8	58.5	56.0	C
		A1+14*A2*B2+2*A6+A36					[331]	
$C_{18}H_{34}O_2$		*trans*-11-octadecenoic acid						
	317	58.49		184.5	171.8	58.5	54.5	
		A1+14*A2*B2+2*A6+A36					[331]	C
$C_{18}H_{34}O_2$		*trans*-12-octadecenoic acid						
	325	56.71		174.5	171.8	56.7	55.8	
		A1+14*A2*B2+2*A6+A36					[331]	C
$C_{18}H_{34}O_2$		*trans*-13-octadecenoic acid						
	318	55.62		174.9	165.2	55.6	52.5	
		A1+11*A2*B2+2*A6+A36+3*A2					[331]	

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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)
$C_{18}H_{34}O_2$		*trans*-14-octadecenoic acid					
	327	57.06		174.5	167.4	57.1	54.7
		$A1+12*A2*B2+2*A6+A36+2*A2$					[331]
$C_{18}H_{34}O_2$		*trans*-15-octadecenoic acid					
	331	58.98		178.2	169.6	59.0	56.1
		$A1+13*A2*B2+2*A6+A36+A2$					[331]
$C_{18}H_{36}$		*cis, cis*-1,3,5-tri-*tert*-butylcyclohexane					
	393.2	26.78		68.1	54.4	26.8	21.4
		$9*A1+A14+3*A15+3*A4+3*A16$					[41]
$C_{18}H_{36}$		*cis, trans*-1,3,5-tri-*tert*-butylcyclohexane					
	338.2	17.99		53.2	54.4	18.0	18.4
		$9*A1+A14+3*A15+3*A4+3*A16$					[41]
$C_{18}H_{38}O_2$		2-(hexadecyloxy)ethanol					
	311.7	14.94	47.93				
	318.5	37.32	117.2	165.1	193.7	52.3	61.7
		$A1+15*A2*B2+A32+A30*B30+2A2$					[88]
$C_{18}H_{38}O_9$		1,ω-dimethoxyocta(oxyethylene)					
	276.2	60.1		217.6	226.4	60.1	62.5
		$2*A1+16*A2*B2+9*A32$					[386]
$C_{18}H_{39}AsO_2$		di-*n*-nonylarsinic acid					
	383	24.3	63.5				
	399	38.1	95.5	159	160	62.4	63.8
		$2*A1+16*A2*B2+A142$					[381]
$C_{18}H_{54}O_9Si_9$		octadecamethylcyclononasiloxane					
	246.2	25.64		104.1	104.2	25.6	25.7
		$18*A12+9*A139+9*A112+A14+15*A15$					[121]
$C_{19}H_{21}F_{19}$*		1,1,1,2,3,3,4,4,5,5,6,6,7,7,8,8-hexadecafluoro-2-(trifluoromethyl)octadecane					
	274.0	1.00	3.65				
	298.0	25.00	83.89	87.54	370.2	26.00	110.3
		$9*A4*B4+6*A25+A27+12*A26+A1+9*A2$					[22]
		Amphiphillic compound					
$C_{19}H_{15}N$*		N-phenyl benzophenone imine					
	392.3	29.14		74.3	76.0	29.14	29.8
		$15*A10+3*A12+A7+A42$					[397]
$C_{19}H_{24}O_3$*		3-[(2,3-dihydro-1H-inden-5-yl)carbonyl]-1,2,2-trimethylcyclopentanecarboxylic acid					
	404.3	22.50		55.7	61.4	22.5	24.8
		$3*A1+2*A14+4*A15+2*A17+A16+2*A19+3*A10+A12+A36*B36+A35$					[366]
$C_{19}H_{26}O_4$		3-(4-methoxy-2,6-dimethylbenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
	416.7	28.31		67.9	82.6	28.3	34.4
		$6*A1+A14+2*A15+2*A17+A16+2*A10+2*A12+2*A11+A36*C36+A35+A32$					[366]
$C_{19}H_{26}O_6$		1,2,2-trimethyl-3-(2,4,6-trimethoxybenzoyl)cyclopentanecarboxylic acid					
	432.2	29.68		68.7	96.2	29.7	41.2
		$6*A1+A14+2*A15+2*A17+A16+2*A10+4*A12+A36*B36$					
		$+A35+3*A32$					[366]
$C_{19}H_{27}NO_3$*		2-[(3,4-dimethylphenyl)(hydroxyimino)methyl]-1,2,2-trimethylcyclopentanecarboxylic					
		acid methyl ester					
	426.0	39.14		91.9	68.6	39.1	29.2
		$6*A1+A14+2*A15+2*A11+A12+3*A10+2*A17+A16+A38+A53+A7$					[373]
$C_{19}H_{27}NO_4$*		3-[(hydroxyimino)(4-ethoxyphenyl)methyl]-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester					
	401.0	36.75		91.65	81.9	36.8	32.8
		$5*A1+A14+2*A15+2*A12+4*A10+2*A17+A16+A38+A32+A2+A7+A53$					[373]
$C_{19}H_{27}NO_5$*		3-[(hydroxyimino)(3,4-dimethoxyphenyl)methyl]-1,2,2-trimethylcyclopentanecarboxylic					
		acid methyl ester					
	393.0	36.20		92.1	82.2	36.2	32.3
		$6*A1+A14+2*A15+3*A12+3*A10+2*A17+A16+A38+2*A32+A7+A53$					[373]
$C_{19}H_{38}O_2$*		ethyl margarate (ethyl heptadecanoate)					
	291.2	16.57	55.5				
	298.4	36.2	115.7	171.2	189.5	52.8	56.6
		$2*A1+A2+15A2*B2+A38$					[391]
$C_{20}H_{13}NO_4$		1-amino-4-hydroxy-2-phenoxy-9,10-anthracenedione					
	458.2	30.79		67.2	82.9	30.8	38.0
		$A14+3*A15+10*A10+4*A12+A31+A45+A32+2*A114+4*A19$					[315]
$C_{20}H_{17}F_{25}$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosafluoroeicosane					
	192	2.4	12.5				
	329	6.1	19.45				
	361	23.7					

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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)
							[17]
	324.2	5.60	17.27				
	355.2	21.90	61.66	78.93	467.7	27.50	166.1
		12*A4*B4+3*A25+22*A26+A1+7*A2					[68]
		Amphiphillic compound (values represent two sets of independent measurements)					
$C_{20}H_{17}N_3O_4$*		4,11-diamino-2-butyl-1H-naphth[2,3-*f*]isoindole-1,3,5,10(2H)-tetraone					
	490.2	24.85		50.69		24.85	
		No prediction made (reporting authors express concern that the enthalpy is too small)					[315]
$C_{20}H_{19}BrS$*		2-*n*-butyl-5-(4-bromobiphenyl-4-yl)thiophene					
	501.4	21.40		42.7	101.5	21.4	50.9
		A1+3*A2+8*A10+4*A12+A21+A14+2*A15+A131+2*A19+2*A18					[14]
$C_{20}H_{21}F_{21}$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-heneicosafluoroeicosane					
	317	4.0	12.62				
	337	24.4	72.38	85.0	186.6	28.4	62.8
							[17]
	306.5	2.20	7.18				
	336.7	26.70	79.30	86.5	186.6	28.9	62.8
		10*A4*B4+3*A25+18*A26+A1+9*A2					[24]
		(Values represent two sets of independent measurements) Amphiphillic compound					
$C_{20}H_{21}F_{19}O$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-nonadecafluoro-10-eicosanone					
	317.9	53.17		167.3	181.4	53.2	57.7
		9*A4*B4+3*A25+16*A26+A35+A1+9*A2					[21]
		Amphiphillic compound					
$C_{20}H_{23}F_{19}O$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-nonadecafluoro-10-eicosanol					
	346.2	3.60	10.40				
	356.0	33.50	94.10	104.5	184.6	37.1	69.2
		9*A4*B4+3*A25+16*A26+A1+9*A2+A30*B30+A3*B3					[23]
-		Amphiphillic compound					
$C_{20}H_{24}$		8-(4-biphenyl)-1-octene					
	291.5	21.00		72.0	107.2	21.0	31.3
		9*A20+2*A12+A11+6*A2+A5+A6					[97]
$C_{20}H_{24}O_6$		dibenzo[18-crown-6]					
	435.75	57.46		131.9	106.1	57.5	44.1
		A14+15*A15+6*A112+4*A19+8*A10					[398]
$C_{20}H_{26}O_3$		1,2,2-trimethyl-3-[(5,6,7,8-tetrahydro-2-naphthalenyl)carbonyl]cyclopentanecarboxylic acid					
	421.3	22.94		54.5	65.1	22.9	27.4
		3*A1+2*A14+5*A15+2*A17+A16+2*A19+3*A10+A12+A36*B36+A35					[366]
$C_{20}H_{28}O_5$		3-(3,4-diethoxybenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
	389.3	29.07		74.7	103.0	29.1	40.1
		5*A1+A14+2*A15+2*A17+A16+4*A10+2*A2+2*A12+A36*C36+A35+2*A32					[366]
$C_{20}H_{32}O_4$		2,5-di-*n*-heptyloxy-1,4-benzoquinone					
	275.8	3.6	13.05				
	372.5	17.3	46.44				
	406.2	38.4	94.53	154.0	140.8	59.3	57.2
		2*A1+12*A2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114					[342]
$C_{20}H_{40}O_2$*		methyl nonadecanoate					
	304.2	19.4	63.7				
	313.2	42.8	136.8	200.5	189.5	62.2	56.6
		2*A1+17*A2*B2+A38					[391]
$C_{20}H_0O_4$		2,2,12,12-tetramethyl-1,3,11,13-tetraoxycycloeicosane					
	369.5	45.60		123.4	102.3	45.6	37.8
		4*A1+A14+17*A15+2*A17+4*A112					[47]
$C_{20}H_{42}O_{10}$		1,ω-dimethoxynona(oxyethylene)					
	289.2	73.9		255.6	249.7	73.9	62.5
		2*A1+18*A2*B2+10*A32					[386]
$C_{20}H_{43}AsO_2$*		di-*n*-decylarsinic acid					
	380	24.5	64.4				
	400	42.3	105.9	170.2	178.6	66.8	71.4
		2*A1+18*A2*B2+A142					[381]
$C_{20}H_{50}Si_5$		decaethylcyclopentasilane					
	254.8	16.3	63.97				
	440.1	1.40	3.18	67.2	114.3	17.7	50.3
		10*A1+10*A2+A14+2*A15+5*A139					[175]
$C_{20}H_{60}O_{10}Si_{10}$		eicosanomethylcyclodecasiloxane					
	265.8	39.76		149.6	113.3	39.8	30.1
		20*A1+10*A139+10*A112+A14+17*A15					[121]
$C_{21}H_{20}BrN_7O_6$		N-[2-[(2-bromo-4,6-dinitrophenyl)azo]-[(2-cyanoethyl)-2-propenylamino]-					

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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-methoxyphenyl] acetamide					
	465.2	59.08		127.0	99.7	59.1	46.4
		4*A10+8*A12+3*A2+2*A1+A5+A6+2*A50+A21+2*A42+A32+A60+A56+A43					[315]
$C_{21}H_{20}N_4O_3$*		4-methoxy-N,N-bis(3-pyridinylmethyl)-1,3-benzenedicarboxamide					
	403.9	28.43		70.4	101	28.4	40.8
		11*A10+2*A11+3*A12+2*A41+2*A2+2*A60+A1+A32					[392]
$C_{21}H_{25}F_{19}$*		1,1,1,2,3,3,4,4,5,5,6,6,7,7,8,8-hexadecafluoro-(trifluoromethyl)eicosane					
	310.1	34.00		109.6	177.7	34.0	55.1
		9*A4*B4+6*A25+A27+12*A26+A1+11*A2					[22]
$C_{21}H_{29}NO_3$*		3-[(hydroxyimino)(5,6,7,8-tetrahydro-2-naphthalenyl)methyl-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester					
	425.0	38.37		90.3	72.5	38.4	30.8
		4*A1+2*A14+5*A15+3*A10+2*A19+2*A17+A12+A16+A38+A7+A53					[373]
$C_{21}H_{30}O$		1,1′-diadamantyl ketone					
	404.7	5.90	14.57				
	470.0	15.70	33.40	48.0	55.0	21.6	25.9
		6*A14+2*A15+6*A16+2*A17+A35					[324]
$C_{21}H_{40}$		*trans*-2-heptyl-6-butyldecalin					
	295.3	31.80		107.7	121.9	31.8	36.0
		2*A14+4*A15+4*A16+2*A1+9*A2					[40]
$C_{21}H_{40}$		*trans*-2-propyl-6-octyldecalin					
	308.8	41.00		133.0	121.9	41.0	37.6
		2*A14+4*A15+4*A16+2*A1+9*A2					[40]
$C_{21}H_{42}O_2$*		ethyl nonadecanoate					
	300.2	18.49	61.6				
	309.2	43.18	139.7	201.3	189.5	61.7	56.6
		2*A1+A2+17*A2*B2+A38					[391]
$C_{21}H_{42}O_2$*		methyl eicosanoate					
	319.2	73.7		231	210	73.7	61.7
		2*A1+18*A2*B2+A38					[391]
$C_{21}H_{43}NO$		N-propylstearamide					
	348.0	16.02	46.03				
	354.0	50.04	141.4	187.4	199.7	66.1	70.7
		2*A1+16*A2*B2+A60+2A2					[291]
$C_{21}H_{43}NO$		N-heptylmyristamide					
	316.0	6.54	20.70				
	343.0	49.02	142.9	163.6	204.1	55.6	70.0
		2*A1+18*A2*B2+A60					[291]
$C_{21}H_{43}NO$		N-decylundecanamide					
	337.0	0.07	0.21				
	344.0	42.45	123.4	123.6	204.1	42.5	70.2
		2*A1+18*A2*B2+A60					[291]
$C_{21}H_{43}NO$		N-laurylnonanamide					
	328.0	0.17	0.52				
	341.0	66.91	196.2	196.7	204.1	67.1	69.6
		2*A1+18*A2*B2+A60					[291]
$C_{21}H_{43}NO$		N-myristylheptanamide					
	313.0	2.08	6.65				
	334.0	52.68	157.7	164.4	204.1	54.8	68.2
		2*A1+18*A2*B2+A60					[291]
$C_{21}H_{43}NO$		N-stearylpropanamide					
	337.0	1.84	5.45				
	350.0	56.03	160.1	165.6	201.9	57.9	70.7
		2*A1+17*A2*B2+A60+A2					[291]
$C_{22}H_{21}F_{25}$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosafluorodocosane					
	207	1.0	4.83				
	342	9.5	27.78				
	365	25.8	70.68	103.3	206.3	36.3	75.3
							[17]
	339.2	7.50	22.11				
	357.2	22.20	62.15	84.26	206.3	29.7	73.7
		12*A4*B4+3*A25+22*A26+A1+9*A2					[68]
		Amphiphillic compound (values represent two sets of independent measurements)					
$C_{22}H_{24}O_3$*		3-([1,1-biphenyl]-4-ylcarbonyl)-1,2,2,-trimethylcyclopentanecarboxylic acid					
	444.2	27.69		62.3	74.6	27.7	33.1
		3*A1+A14+2*A15+2*A17+A16+9*A10+3*A12+A36*B36+A35					[366]
$C_{22}H_{25}F_{21}$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-heneicosofluorodocosane					
	334.1	6.00	17.96				
	338.1	27.00	79.86	97.8	200.8	33.0	67.9

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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)
	10*A4*B4+18*A26+3*A25+A1+11*A2					[22]
	Amphiphillic compound					
$C_{22}H_{26}N_2O_2$	(4R, 4′R, 5R, 5′R)-5,5-diphenyl-3,3′,4,4′-tetramethyl-2,2′-bioxazolidine					
394.0	31.9		81.0	82.4	31.9	32.5
	2*A14+4*A15+2*A112+2*A119+6*A16+4*A1+10*A10+2*A11					[387]
$C_{22}H_{26}N_2O_2$	(2R, 3R, 6R, 7R)-2,6-diphenyl-3,4,7,8-tetramethyl-cis-perhydro-[1,4]-oxazino-[3,2-*b*]-[1,4]-oxazine					
379.4	18.4		48.5	82.4	18.4	31.3
	2*A14+4*A15+2*A112+2*A119+6*A16+4*A1+10*A10+2*A11					[387]
$C_{22}H_{28}N_2O$	N-phenyl-N-[1-(2-phenylethyl)-4-piperidinyl]propanamide (fentanyl)					
357.2	22.51		63.0	84.6	22.5	30.2
	A14+3*A15+A16+A119+3*A2+10*A10+A11+A12+A1+A125					[296]
$C_{22}H_{29}NO_2$	4-*n*-octyloxy-N-(4-methoxybenzylidene)aniline					
377.3	42.29		112.1	127.0	42.3	47.9
	2*A1+7*A2+2*A32+8*A10+4*A12+A6+A42					[141]
$C_{22}H_{30}N_2O_2S$	N-[4-(methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidinyl]-N-phenylpropanamide (sufentanil)					
370.2	23.85		64.4	102.3	23.9	37.9
	2*A14+5*A15+A17+A119+A59+5*A10+A12+2*A1+4*A2+A32+2*A18+A18*B18+A19+A131					[296]
$C_{22}H_{36}O_4$	2,5-di-*n*-octyloxy-1,4-benzoquinone					
358.2	9.4	26.24				
405.8	43.0	106.0	132.2	155.0	52.4	62.9
	2*A1+14*A2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114					[342]
$C_{22}H_{40}O_2$	3,3,6,6,10,10,13,13-octamethylcyclotetradecane-1,8-dione					
492.2	24.7		50.2	73.7	24.7	36.3
	8*A1+4*A17+2*A114+A14+11*A15					[115]
$C_{22}H_{46}O$	1-docosanol					
333.9	17.24	50.72				
345.2	46.57	134.9	185.6	214.6	63.8	74.08
	A1+21*A2*B2+A30					[88]
$C_{22}H_{47}AsO_2$*	di-*n*-undecylarsinic acid					
384	30.0	78.2				
396	45.1	113.9	192.1	197.2	75.1	78.1
	2*A1+20*A2*B2+A142					[381]
$C_{22}H_{66}O_{11}Si_{11}$	docosamethylcycloundecasiloxane					
216.2	17.73		82.0	122.4	17.7	26.5
	22*A1+11*A139+11*A112+A14+19*A15					[121]
$C_{23}H_{24}N_6O_4$	2-[[4-[[(2-acetoxy)ethyl]butylamino]-2-methylphenyl]azo]-5-nitro-1,3-benzenedicarbonitrile					
424.2	37.88		89.3	105.7	37.9	44.8
	5*A10+6*A12+A11+2*A56+A50+3*A1+5*A2+2*A42+A43+A38					[315]
$C_{23}H_{25}BrN_6O_{10}$	N-[5-[bis[(2-acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-methoxyphenyl]acetamide					
421.2	57.28		136.0	117.1	57.3	49.3
	4∗A10+8∗A12+4∗A1+4∗A2+2∗A38+A21+2∗A50+2∗A42+A32 +A60+A43					[315]
$C_{23}H_{31}NO$	4-*n*-octyloxy-N-(3,5-dimethylbenzylidene)aniline					
324.7	37.7		116.2	120.8	37.7	39.2
	3*A1+7*A2+A32+7*A10+2*A11+3*A12+A6+A42					[141]
$C_{23}H_{31}NO_3$	4-*n*-octyloxy-N-(3,5-dimethoxybenzylidene)aniline					
316.3	35.3		111.6	134.4	35.3	42.5
	3*A1+7*A2+3*A32+7*A10+5*A12+A6+A42					[141]
$C_{23}H_{44}$	*trans*-2-heptyl-6-hexyldecalin					
312.2	38.9		124.6	136.1	38.9	42.5
	2*A1+4*A15+4*A16+2*A1+11*A2					[40]
$C_{23}H_{44}$	*trans*-2-pentyl-6-octyldecalin					
314.2	43.5		138.5	136.1	43.5	42.8
	2*A1+4*A15+4*A16+2*A1+11*A2					[40]
$C_{23}H_{46}O_2$*	methyl behenate (methyl docosanoate)					
327.2	82.3		231	210	82.3	67.1
	2*A1+20A2*B2+A38					[391]
$C_{24}H_{18}N_2S_2$*	4,4′-bis-(2-thienylmethylidenamino)-*trans*-stilbene					
567.2	44.90	79.16				
580.2	0.20	0.34	79.5		45.1	
	No prediction made (forms liquid crystal)					[86]
$C_{24}H_{18}N_2S_2$*	1,2-bis-[5-(β-azastyryl)-2-thienyl]-*trans*-ethylene					
501.2	45.90		91.6	108.4	45.9	54.3
	10*A10+2*A12+4*A6+2*A42+2*A14+4*A15+4*A18+4*A19+2*A131					[86]
$C_{24}H_{25}F_{25}$*	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluorotetracosane					

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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)
	352.1	10.00	28.40				
	364.1	26.00	71.41	99.8	220.5	36.0	80.3
		12*A4*B4+3*A25+22*26+A1+11*A2					
		Amphiphillic compound					[22]
$C_{24}H_{25}F_{25}$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluoro-14-methyltricosane					
	220.0	9.00	34.61				
	347.1	25.00	72.02	106.6	207.5	34.0	72.0
		12*A4*B4+3*A25+22*A26+2*A1+A3+9*A2					
		Amphiphillic compound					[22]
$C_{24}H_{30}O_4$		2,2′-diphenyl-bi(5,5-dimethyl-1,3-dioxan-2-yl)					
	507.1	49.8		98.2	80.6	49.8	40.9
		2*A14+6*A15+4*A17+4*A112+10*A10+2*A11+4*A1					[385]
$C_{24}H_{32}$*		8-[4-(4′-*n*-butylbiphenyl)]-1-octene					
	248.6	2.20	8.85				
	315.6	9.60	30.4	39.3	129.1	11.8	40.7
		8*A10+2*A12+2*A11+A5+A6+A1+9*A2					[97]
		Forms liquid crystal					
$C_{24}H_{40}O_4$		2,5-di-*n*-nonyloxy-1,4-benzoquinone					
	352.6	8.0	22.69				
	383.8	24.2	63.05				
	402.7	47.1	117.0	202.7	169.2	79.3	68.1
		2*A1+16*A2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114					[342]
$C_{24}H_{40}O_8$		dibenzo[24-crown-8]					
	354.1	16.6	46.9				
	375.4	52.25	139.2	186.1	130.1	68.85	49.1
		A14+15*A15+6*A112+4*A19+8*A10					[398, 399]
$C_{24}H_{44}$		*trans*-2,6-diheptyldecalin					
	326.7	40.17		123.0	143.2	40.2	46.8
		2*A1+4*A15+4*A16+2*A1+11*A2					[40]
$C_{24}H_{44}O_2$		3,3,7,7,11,11,15,15-octamethylcyclohexadecane-1,9-dione					
	423.2	34.30		81.0	81.1	34.3	34.3
		8*A1+4*A17+2*A114+A14+13*A15					[115]
$C_{24}H_{50}O_2$*		2-(docosanoxy)ethanol					
	317.2	12.92	40.73				
	335.9	43.93	130.8	171.5	249.5	56.9	83.8
		A1+21*A2*B2+A32+A30*B30					[88]
$C_{24}H_{51}AsO_2$*		di-*n*-dodecylarsinic acid					
	385	31.4	81.5				
	398	49.4	124.1	205.7	215.8	80.8	85.9
		2*A1+22*A2*B2+A142					[381]
$C_{24}H_{72}O_{12}Si_{12}$		tetracosamethylcyclododecasiloxane					
	234.2	15.45		65.97	131.5	15.5	30.8
		24*A1+12*A139+12*A112+A14+21*A15					[121]
$C_{26}H_{22}N_2O_2S_2$*		1,2-bis-[5-(4-methoxy-β-azastyryl)-2-thienyl]-*trans*-ethylene					
	538.2	63.50	118.0				
	567.2	0.80	1.41	119.4	123.2	64.30	69.88
		2*A1+8*A10+4*A12+4*A6+2*A42+2*A14+4*A15+4*A18+4*A19+2*A131+2*A32					
		Forms liquid crystal					[86]
$C_{26}H_{29}F_{25}$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosafluorohexacosane					
	363	16.3	44.90				
	366	26.1	71.31	116.2		42.4	
							[17]
	359.2	26.0	72.38			26.0	
		Amphiphillic compound (values represent two sets of independent measurements)					[68]
$C_{26}H_{42}O$*		*trans*-1-(4-heptanoylphenyl)-4-heptylcyclohexane					
	343.2	16.49	48.05				
	344.7	7.71	22.37	70.4	145.5	24.2	50.2
		A14+3*A15+2*A16+4*A10+A11+A12+2*A1+11*A2+A35					[25]
		Forms liquid crystal					
$C_{26}H_{48}O_2$		4,4,7,7,13,13,16,16-octamethylcyclooctadecane-1,10-dione					
	492.2	50.60		102.8	88.5	50.6	43.6
		8*A1+4*A17+2*A114+A14+15*A15					[115]
$C_{26}H_{54}O$		1-hexacosanol					
	332.2	16.74	50.39				
	351.7	67.78	192.7	243.1	251.8	84.5	88.6
		A1+25*A2*B2+A30					[78]

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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)
$C_{26}H_{55}AsO_2$*		di-*n*-tridecylarsinic acid					
	388	36.5	94.0				
	396	52.7	133.1	227.2	234.4	89.2	92.8
		2*A1+24*A2*B2+A142					[381]
$C_{27}H_{42}Cl_2N_2O_6$*		chloramphenicol palmitate polymorph A					
	367.3	51.04	0	139	188.6	51.04	69.2
		chloramphenicol palmitate polymorph B					
	360.8	41.3	0	112.5	188.6	41.3	69.2
		4*A10+A11+A12+A50+A30*F30+2*A22*F22+A60+A38+A2+3*A3*B3+					
		A1+14*A2					[395]
$C_{28}H_{22}N_2O_2$		1,4-[bis[(4-methylphenyl)amino]-9,10-anthracenedione					
	491.2	36.59		74.5	71.5	36.6	35.1
		3*A15+A14+14*A10+4*A19+2*A114+4*A12+2*A1+2*A11+2*A44					[315]
$C_{28}H_{31}F_{25}$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluorooctacosane					
	263.2	43.10		163.8	248.9	43.10	65.5
		12*A4*B4+3*A25+22*A26+A1+15*A2					[68]
		Amphiphillic compound					
$C_{28}H_{48}O$*		*trans*-1-heptyl-4-(4-nonanoylphenyl)cyclohexane					
	343.4	20.8	60.6				
	353.3	11.32	32.1	92.6	159.7	32.1	56.4
		A14+3*A15+2*A16+4*A10+A11+A12+2*A1+13*A2+A35					
		Forms liquid crystal					[25]
$C_{28}H_{48}O_4$		2,5-di-*n*-undecyloxy-1,4-benzoquinone					
	367.4	12.9	35.11				
	390.0	28.4	72.8				
	397.2	52.1	131.2	239.1	241.6	93.4	96.0
		2*A1+20*A2*B2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114					[342]
$C_{28}H_{52}O_2$		4,4,8,8,14,14,18,18-octamethylcycloeicosane-1,11-dione					
	418.2	36.80		88.0	95.9	36.8	40.1
		8*A1+4*A17+2*A114*+A14+17*A15					[115]
$C_{28}H_{59}AsO_2$*		di-*n*-tetradecylarsinic acid					
	390	39.3	100.6				
	397	58.2	146.6	247.2	253.0	97.5	100.5
		2*A1+26*A2*B2+A142					[381]
$C_{29}H_{41}NO_4$		17-(cyclopropylmethyl)-α-(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy-α-methyl-6,14-ethenomorphinan-7-methanol					
	491.3	26.80		54.55	68.6	26.80	33.7
		6*A14+2*A15+5*A1+2*A4+A30*E30+4*A16+3*A17+A119+A112+A31+A32+					
		3*A19+A12+2*A10+A2					[320]
$C_{30}H_{37}F_{25}$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluorotricontane					
	365.2	47.80		130.9	263.1	47.80	96.1
		12*A4*B4+3*A25+22*A26+A1+17*A2					[68]
$C_{30}H_{56}O_2$		5,5,8,8,16,16,19,19-octamethylcyclodocosane-1,12-dione					
	442.2	47.70		107.9	95.9	47.7	42.4
		8*A1+4*A17+2*A114+A14+17*A15					[115]
$C_{30}H_{60}O_{15}$		45-crown-15					
	311.2	70.6		227	206.8	70.6	64.3
		A14+42*A15+15*A112					[386]
$C_{30}H_{63}AsO_2$*		di-*n*-pentadecylarsinic acid					
	390	46.4	119				
	396	63.6	160.5	279.6	271.6	110.0	107.6
		2*A1+28*A2*B2+A142					[381]
$C_{31}H_{43}NO_5$		3-(acetyloxy)-17-(cyclopropylmethyl)-α-(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy-α-methyl-6,14-ethenomorphinan-7-methanol					
	440.3	22.40		50.9	68.9	22.4	30.3
		6*A14+2*A15+6*A1+2*A4+A30*E30+4*A16+3*A17+A119+A112+					
		3*A19+A12+2*A10+A2+A38					[320]
$C_{32}H_{34}$		1,8-bis-(4-biphenyl)octane					
	415.2	56.00		134.9	140.8	56.0	58.5
		18*A10+4*A12+2*A11+8*A2					[97]
$C_{32}H_{34}$*		1,8-bis[4(4′-ethylbiphenyl)]butane					
	454.2	46.00		101.3	127.8	46.0	58.1
		2*A1+6*A2+16*A10+4*A12+4*A11					[97]
$C_{32}H_{41}F_{25}$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluorodotriacontane					
	369.2	43.40		117.6	277.3	43.4	102.3
		12*A4*B4+3*A25+22*A26+A1+19*A2					[68]
$C_{32}H_{64}16$		48-crown-16					
	312.2	59.1		189.4	219.1	59.1	68.4
		A14+45*A15+16*A112					[386]

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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)
$C_{32}H_{45}NO_5$		17-(cyclopropylmethyl)-α-(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy-α-methyl-(1-oxopropoxy)-6,14-ethenomorphinan-7-methanol					
	410.2	27.10		66.07	76.0	27.10	31.2
		6*A14+2*A15+6*A1+2*A4+A30*E30+4*A16+3*A17+A119+A112+3*A19+A12+2*A10+2*A2+A38					
$C_{32}H_{60}O_2$		5,5,9,9,17,17,21,21-octamethylcyclotetracosane-1,13-dione					[320]
	380.2	32.60		85.7	110.7	32.6	42.1
		8*A1+4*A17+2*A114+A14+21*A15					[115]
$C_{32}H_{67}AsO_2$*		di-*n*-hexadecylarsinic acid					
	389	47.4	121.9				
	395	66.8	169.2	291	290.2	114.2	114.6
		2*A1+30*A2*B2+A142					[381]
$C_{33}H_{47}NO_5$		17-(cyclopropylmethyl)-α-(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy-α-methyl-(1-oxobutoxy)-6,14-ethenomorphinan-7-methanol					
	422.1	32.40		76.76	83.1	32.40	35.1
		6*A14+2*A15+6*A1+2*A4+A30*E30+4*A16+3*A17+A119+A112+3*A19+A12+2*A10+3*A2+A38					
$C_{34}H_{31}ClN_2O_3$*		spiro[isobenzofuran-1(3H),9′(9H)-7′-chloro-6′-(methylcyclohexylamino)-3′-methyl-2′-anilinoxanthene]-3-one					[320]
	442.2	49.0		110.8	91.5	49.0	40.5
		3*A14+8*A15+2*A1+13*A10+4*A12+A11+6*A19+A16+A17+A112+A115+A43+A44+A22*E22					
$C_{34}H_{32}N_2O_3$		spiro[isobenzofuran-1(3H),9′(9H)-6′-(methylcyclohexylamino)-3′-methyl-2′-anilinoxanthene]-3-one					[371]
	476.2	39.9		83.8	90.2	39.9	43.0
		3*A14+8*A15+2*A1+14*A10+3*A12+A11+6*A19+A16+A17+A112+A115+A43+A44					
$C_{34}H_{38}$*		1,6-*bis*-[4-(4′-ethylbiphenyl)]hexane					[371]
	393.2	3.90	9.92				
	422.2	35.00	82.90	92.83	142.0	38.9	60.0
		2*A1+8*A2+16*A10+4*A11+4*A12					[97]
$C_{34}H_{49}NO_5$		17-(cyclopropylmethyl)-α-(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy-α-methyl-(1-oxopentoxy)-6,14-ethenomorphinan-7-methanol					
	379.1	24.00		63.31	90.2	24.0	34.2
		6*A14+2*A15+6*A1+2*A4+A30*E30+4*A16+3*A17+A119+A112+3*A19+A12+2*A10+4*A2+A38					
$C_{34}H_{68}O_{17}$		51-crown-17					[320]
	301.2	66.6		221.1	231.4	66.6	69.7
		A14+48*A15+17*A112					[386]
$C_{34}H_{71}AsO_2$*		di-*n*-octadecylarsinic acid					
	390	50.9	130.6				
	393	68.6	174.5	305.1	308.8	119.5	121.4
		2*A1+32*A2*B2+A142					[381]
$C_{35}H_{51}NO_5$		17-(cyclopropylmethyl)-α-(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy-α-methyl-(1-oxohexyloxy)-6,14-ethenomorphinan-7-methanol					
	352.6	22.60		64.1	97.3	22.6	35.0
		6*A14+2*A15+6*A1+2*A4+A30*E30+4*A16+3*A17+A119+A112+3*A19+A12+2*A10+5*A2+A38					
$C_{36}H_{42}$*		1,8-*bis*-[4-(4′-ethylbiphenyl)]octane					[320]
	402.2	8.40	20.89				
	413.2	42.00	101.6	122.5	156.2	50.4	64.5
		2*A1+16*A10+4*A12+4*A11+10*A2					[97]
$C_{36}H_{42}$*		1,4-*bis*-[4-(4′-*n*-butylbiphenyl)]butane					
	404.2	12.00	29.68				
	464.2	24.00	51.70	81.3	142.0	36.0	60.0
		2*A1+16*A10+4*A12+4*A11+10*A2					[97]
		Forms liquid crystal					
$C_{36}H_{53}NO_5$		17-(cyclopropylmethyl)-α-(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy-α-methyl-(1-oxoheptyloxy)-6,14-ethenomorphinan-7-methanol					
	360.0	19.30		53.61	104.4	19.30	37.6
		6*A14+2*A15+6*A1+2*A4+A30*E30+4*A16+3*A17+A119+A112+3*A19+A12+2*A10+6*A2+A38					
$C_{36}H_{64}O_4$		2,5-di-*n*-pentadecyloxy-1,4-benzoquinone					[320]
	385.9	21.7	56.23				
	393.5	101.7	258.5	314.7	316.0	123.4	124.3
		2*A1+28*A2*B2+A14+3*A15+2*A18+2*A19+2*A32+2*A14					[342]
$C_{36}H_{74}O_{16}$		54-crown-18					
	317.2	81.6		257.2	243.7	81.6	77.3

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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+51**A*15+18**A*112					[386]
$C_{36}H_{74}O_{18}$		1,ω-dimethoxyheptadeca(oxyethylene)					
	301.2	136.6		453.5	436.2	136.6	131.4
		2**A*1+34**A*2**B*2+18**A*32					[386]
$C_{36}H_{75}AsO_2$*		di-*n*-nonadecylarsinic acid					
	394	128.9		327.2	327.4	128.9	129.0
		2**A*1+34**A*2**B*2+*A*142					[381]
$C_{38}H_{68}O_4$		2,5-di-*n*-hexadecyloxy-1,4-benzoquinone					
	357.7	6.8	18.73				
	370.9	14.1	38.02				
	389.0	19.0	48.84				
	394.2	83.0	210.6	316.1	334.6	122.9	133.0
		2**A*1+30**A*2**B*2+*A*14+3**A*15+2**A*18+2**A*19+2**A*32+2**A*114					[342]
$C_{38}H_{78}O_{19}$		1,ω-dimethoxyoctadeca(oxyethylene)					
	305.2	156.7		513.5	459.5	156.7	140.2
		2**A*1+36**A*2**B*2+19**A*32					[386]
$C_{40}H_{40}N_2O_4$*		3,3′,4,4′-biphenyltetracarboxy-N,N′-bis-(4-*n*-hexylphenyl)diimide					
	432.4	19.9	46.02				
	513.8	26.2	50.99				
	563.3	9.50	16.86	113.9		55.60	
		No prediction made. Forms liquid crystal					[87]
$C_{40}H_{50}$*		1,8-*bis*[4(4′-*n*-butylbiphenyl)]octane					
	398.2	13.0	32.65				
	414.2	27.0	65.19	97.2	184.6	40.0	76.5
		2**A*1+16**A*10+4**A*12+4**A*11+14**A*2					[97]
		Forms liquid crystal					
$C_{40}H_{72}O_4$		2,5-di-*n*-heptadecyloxy-1,4-benzoquinone					
	383.6	13.0	33.89				
	395.3	120.9	305.8	339.7	353.1	133.9	139.6
		2**A*1+32**A*2**B*2+*A*14+3**A*15+2**A*18+2**A*19+2**A*32+2**A*114					[342]
$C_{42}H_{44}N_2O_4$*		3,3′,4,4′-biphenyltetracarboxy-N,N′-bis-(4-*n*-heptylphenyl)diimide					
	411.0	18.80	45.74				
	504.9	24.70	48.92				
	560.8	11.10	19.79	114.5		54.6	
		Forms liquid crystal					[87]
$C_{44}H_{48}N_2O_4$*		3,3′,4,4′-biphenyltetracarboxy-N,N′-bis-(4-*n*-octylphenyl)diimide					
	428.5	36.10	84.25				
	499.2	21.30	42.67				
	553.5	8.50	15.36	142.3		65.9	
		Forms liquid crystal					[87]
$C_{44}H_{80}O_4$		2,5-di-*n*-nonadecyloxy-1,4-benzoquinone					
	385.5	16.2	42.0				
	396.2	134.0	338.2	380.2	390.5	150.2	154.7
		2**A*1+36**A*2**B*2+*A*14+3**A*15+2**A*18+2**A*19+2**A*32+2**A*114					[342]
$C_{44}H_{90}$		*n*-tetratetracontane					
	360.9	145.5		403.1	425.8	145.5	153.7
		2**A*1+42**A*2**B*2					[210]
$C_{50}H_{102}$		*n*-pentacontane					
	366.9	185.0		504.2	481.6	185.0	176.7
		2**A*1+48**A*2**B*2					[210]
$C_{52}H_{106}O_{26}$		1,ω-dimethoxypentacosa(oxyethylene)					
	316.2	209.7		663.3	622.7	209.7	196.9
		2**A*1+50**A*2**B*2+26**A*32					[386]
$C_{54}H_{108}O_{27}$		81-crown-27					
	314.2	155.6		495.4	354.4	155.6	111.3
		*A*14+78**A*15+27**A*112					[386]
$C_{56}H_{114}O_{28}$		1,ω-dimethoxyheptacosa(oxyethylene)					
	315.2	224.6		712.6	669.3	224.6	210.9
		2**A*1+54**A*2**B*2+28**A*32					[386]
$C_{92}H_{186}O_{46}$		1,ω-dimethoxypentatetracosa(oxyethylene)					
	324.2	374.8		1156.3	1089.0	374.8	353.0
		2**A*1+90**A*2**B*2+46**A*32					[386]
$C_{100}H_{202}$		*n*-hectane					
	365.5	54.8	149.9				
	388.5	331.8	854.1	1004.0	946.7	386.8	368.8
		2**A*1+98**A*2**B*2					[343]
$C_{192}H_{386}$		*n*-dononacontahectane					

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—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)
399.1	698.9		1751.2	1802.4	698.9	719.3 [344]
2*A1+190*A2*B2 (Authors noted a small premelting transition)						

[a]Units for $\Delta_0^{T_{fus}} S_{tpce}$ and $\Delta_0^{T_{fus}} H_{tpce}$ are $J \cdot mol^{-1} \cdot K^{-1}$ and $kJ \cdot mol^{-1}$, respectively; compounds with molecular formulas characterized with an asterisk(*) were not included in generating the statistics. As noted in the table, some of these compounds exhibit liquid crystal behavior, others display amphiphillic behavior, group values for some are not currently available, the error between experimental and calculated total phase change entropy exceeded three standard deviations or some may have been added at a later date.