

Appendix A
Supplementary Material

Total Phase Change Entropies and Enthalpies. An update on Fusion Enthalpies and Their Estimation

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Table A1. Experimental and Calculated Molar Transition Enthalpies (ΔH_{pce}), Total Phase Change Enthalpies ($\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$) in $\text{kJ}\cdot\text{mol}^{-1}$, Phase Change Entropies (ΔS_{pce}), and Total Phase Change Entropies $\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ in $\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ of Organic and Organometallic Compounds

Compound	T (K)	ΔH_{pce} Calculation	ΔS_{pce} exp	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ exp	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ calc	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ exp	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ calc
GeI ₂	701.2	germanium diiodide 33.3	0	47.5		33.3	
		prediction not made					[304]
C ₂ HCl ₂ F ₃	145.7	1,1,1-trifluoro-2,2-dichloroethane 5.51	0	37.8	39.2	5.51	5.7
		2*A22*D22+3*A25+A4*B4+A3*B3					[7]
C ₂ H ₃ BrO ₂	319.2	bromoacetic acid 13.9	0	43.5	40.8	13.9	13.0
		A21+A2+A36*B36					[104]
C ₂ H ₃ ClO ₂	334.8	chloroacetic acid 16.3	0	48.7	39.5	16.3	13.2
		A22*D22+A2+A36*B36					[104]
C ₂ H ₃ IO ₂	355.1	iodoacetic acid 15.5	0	43.7	42.7	15.5	15.2
		A29+A2+A36*B36					[104]
C ₂ H ₄ N ₂ O ₂	356.2	oxamide 1.88	5.28				
	455.5	3.56	7.82				
	494.3	6.24	12.63	25.7	42.8 ^a	11.7	21.1

	Decomposed prior to melting 2*A45						[357]
C ₂ H ₆ N ₂ O	1-methyl urea						
372.0	12.5	0	33.6	31.7	12.5	11.8	
	A1+A67						[305]
C ₃ H ₂ N ₂	malononitrile						
260.9	0.43	1.65					
305.0	10.70	35.08	36.7	42.5	11.1	13.0	
	A2+2*A56						[402]
C ₃ H ₂ N ₂ O ₃	imidazolidine-2,4,5-trione						
392.3	2.1	5.35		44.8 ^a		22.3	
520.0	Compound decomposed on melting						
	A14+2*A15+A124*2+A114						[423]
C ₃ H ₄ N ₄ O ₆	1,3,3-trinitroazetidide						
373.8	29.0	0	77.6	48.6	29.0	18.2	
	A14+A15+A120+2*A50+A17						[192]
C ₃ H ₄ O ₃	ethylene carbonate						
311.2	13.0	0	41.8	42.1	13.0	13.1	
	A14+2*A15+A116						[154]
C ₃ H ₄ O ₄	malonic acid						
407.5	23.1	0	56.7	39.5	23.1	16.1	
	A2+2*A36*B36						[215]
C ₃ H ₅ NO ₂	dimethylene urethane						
360.0	17.3	0	48.1	56.1	17.3	20.2	
	A14+2*A15+A154						[163]
C ₃ H ₅ NOS	2-mercapto-2-oxazoline						
370.0	15.9	0	43.0	43.4	15.9	16.1	
	A14+2*A15+A163						[387]
C ₃ H ₅ NS	2-mercapto-2-thiazoline						
377.0	16.8	0	44.6	44.6	16.8	16.8	
	A14+2*A15+A165						[387]

C ₃ H ₆ N ₂ O	2-imidazolidinone						
344.6	3.6	10.45					
401.2	11.5	28.66	39.11	47.3	15.1	19.0	
	A14+3*A15+A129						[411]
C ₃ H ₆ N ₂ O ₂	malonamide						
418.9	1.89	4.51					
444.2	29.85	67.20	71.71	62.9	31.74	27.9	
	2*A61+A2						[357]
C ₃ H ₆ O ₃	dimethyl carbonate						
220.1	Not reported						
278.2	11.58	41.62	28.1	42.2	11.58	7.8	
	2*A1+A149						[154]
C ₃ H ₆ S ₃	1,3,5-trithiane						
488.4	32.2	0	65.9	53.2	32.3	26.0	
	A14+3*A15+3*A131						[10]
C ₃ H ₇ NO	propanamide						
352.6	12.9	0	36.6	52.6	12.9	18.5	
	A1+A2+A61						[391]
C ₃ H ₇ NO	N,N-dimethylformamide						
212.9	8.95	0	42.0	42.1	8.95	9.0	
	2*A1+A62						[400]
C ₃ H ₈ N ₂ O	1-ethyl urea						
356.7	9.6	0	26.9	38.8	9.6	13.8	
	A1+A2+A67						[305]
	[Note: Compound in database – this value is quite a bit lower than previously reported]						
C ₃ H ₈ O	1-propanol						
148.7	5.40	0	36.3	33.5	5.40	5.00	
	A1+2*A2+A30						[187]
C ₃ H ₉ NO	3-amino-1-propanol						
284.1	16.9	0	59.5	67.0	16.9	19.0	
	3*A2*B2+A45+A30*B30						[137]
C ₃ H ₁₀ N ₂	propane-1,3-diamine						

	260.6	10.53	40.41					
	262.4	12.19	46.46	86.9	70.7	22.72	18.6	
		3*A2*B2+2*A45						[15]
C ₄ F ₆ N ₂ S		3,4-bis(trifluoromethyl)-1,2,5-thiadiazole						[71148-78-2]
	284.0	11.5	0	40.5	54	11.5	15.3	
		A14+2*A15+A131+2*A118+2*A4*B4+6*A25+2*A19						[63]
C ₄ H ₂ Cl ₂ S		2,5-dichlorothiophene						
	232.7	11.87	0	51.0	48.3	11.87	11.2	
		A14+2*A15+2*A22*D22+A131+2*A18+2*A19						[372]
C ₄ H ₃ ClS		3-chlorothiophene						
	214.2	9.39	0	43.8	39.9	9.39	8.5	
		A14+2*A15+A22*D22+A131+A18+2*A18*B18+A19						[233]
C ₄ H ₄ N ₂		pyrazine						
	300.5	1.09	3.63					
	309.8	0.05	0.16					
	325.4	14.78	45.42	49.2	51.4	15.92	16.7	
		4*A10+2*A41						[140]
		[Note: Compound is already in published data base; however, the earlier data did not report values for the two solid to solid phase transitions. The earlier enthalpy of fusion value was also considerably smaller.						
C ₄ H ₄ N ₂		succinonitrile						
	233.6	6.09	26.07					
	330.3	3.75	11.35	37.4	49.6	9.84	16.4	
		2*A56+2*A2						[402]
C ₄ H ₄ N ₂ O ₃		Barbituric acid						
	516.0	1.30	2.52					
	526.4	20.87	39.65	42.2	49.5	22.17	26.1	
		A14+3*A15+A129+A121						[447]
C ₄ H ₆ F ₄ O ₂		1,2-dimethoxytetrafluoroethane						
	252.0	10.75	0	42.7	51.5	10.75	13.0	
		2*A1+2*A32+4*A26+2*A4*B4						[320]
C ₄ H ₆ O ₃		propylene carbonate						
	220.3	8.96	0	40.7	45.0	8.96	9.9	

								2*A15+A14+A1+A16*B16+A116	[154]
C ₄ H ₆ O ₄	1,4-butanedioic acid (succinic acid)								
455.2	34.0	0	74.7	51.0	34.0	23.2			
								2*A36*B36+2*A2*B2	[298]
C ₄ H ₇ NOS	tetrahydro-2H-1,3-oxazine-2-thione								
400.2	18.4	0	46.0	47.1	18.4	18.8			
								A14+3*A15+A163	[387]
C ₄ H ₇ NO ₂	(R)-4-hydroxy-2-pyrrolidone								
392.0	23.41	0	59.7	61.2	23.4	24.0			
								A14+2*A15+A124+A30*B30	[214]
C ₄ H ₈ N ₂ O ₂	succinamide								
485.9	6.08	12.51		74.4		36.2			
								Decomposed prior to melting	
								2*A2+2*A61	[357]
C ₄ H ₈ N ₄ O ₄	1,4-dinitropiperizine								
489.2	200.8	0	410.5	74.4 ^a	200.8	32.2			
								Note: Enthalpy of fusion is abnormally large – compound may be decomposing	
								A14+3*A15+2*A120+2*A51	[103]
C ₄ H ₈ OS ₂	1,3-dithiane sulfoxide								
361.9	22.6	0	62.45	62.5	22.6	22.6			
								A164+A14+A15*3+A131	[145]
C ₄ H ₈ O ₂ S ₂	1,3-dithiane sulfone								
414.0	22.0	0	53.1	45.2	22.0	18.7			
								Independent value from another reference	
413.8	23.47	0	56.7	45.2	23.47	18.7			
								A14+3*A15+A131+A134	[145,195]
C ₄ H ₈ O ₂ S ₂	1,4-dithiane sulfone								
474.2	26.0	0	54.8	45.2	26.9	21.4			
								A14+3*A15+A131+A134	[347]
C ₄ H ₈ O ₃	ethyl methyl carbonate								
219.4	11.24	0	51.2	35.2	11.24	7.7			
								2*A1+A2+A149	[154]

C ₄ H ₈ O ₃ S	1,3-oxathiane sulfone						
352.9	15.2	0	43.1	43.5	15.2	15.4	
	A14+3*A15+A112+A134						[347]
C ₄ H ₈ O ₃ S	1,4-oxathiane sulfone						
403.3	20.2	0	50.09	43.5	20.2	17.5	
	Note: Enthalpy of fusion value contains an unresolved solid-solid phase transition enthalpy A14+3*A15+A112+A134						[347]
C ₄ H ₉ NO	N,N-dimethylacetamide						
254.2	10.20	0	40.1	41.6	10.20	10.6	
	3*A1+A59						[400]
C ₄ H ₉ NO	butanamide						
387.3	19.2	0	49.6	64.1	19.2	24.8	
	A1+2*A2*B2+A61						[391]
C ₄ H ₉ NO	2-methylpropanamide						
400.1	19.2	0	48.0	53.3	19.2	21.3	
	2*A1+A3*B3+A61						[391]
C ₄ H ₁₀ N ₂ O	1-propyl urea						
291.3	2.4	8.24					
370.2	11.9	32.14	40.4	50.0	14.3	18.6	
	2*A2*B2+A1+A67						[305]
C ₄ H ₁₀ O ₂	meso 2,3-butanediol						
306.6	10.8	0	35.2	50.8	10.8	15.6	
	2*A1+2*A3*B3+2*A30*B30						[125]
C ₄ H ₁₀ O ₂ S ₂	meso 1,2-bis(methylsulfinyl)ethane						
446.7	34.31	0	76.8	65.4	34.31	29.2	
	2*A1+2*A2+2*A87						[119]
C ₄ H ₁₀ O ₂ S ₂	racemic 1,2-bis(methylsulfinyl)ethane						
405.4	22.18	0	54.7	65.4	31.5	26.5	
	[Note: The enthalpy and entropy of fusion values given in the paper are not consistent] 2*A1+2*A2+2*A87						[119]

C ₄ H ₁₀ O ₄	erythritol						
391.2	38.9	0	99.4	83.6	38.9	32.7	[324]
	2*A2+2*A3*B3+4*A30*D30						
C ₄ H ₁₀ O ₄	L-threitol						
361.8	29.1	0	80.43	83.6	29.1	30.2	[324]
	2*A2+2*A3*B3+4*A30*D30						
C ₄ H ₁₂ N ₂	butane-1,4-diamine						
295.1	28.06	0	95.1	80.0	28.06	23.6	[15]
	4*A2*B2+2*A45						
C ₅ H ₂ N ₄ O ₆	2,4,6-trinitropyridine						
436.2	22.0	0	50.4	56.3	22.0	24.6	[272]
	2*A10+3*A12+A41+3*A50						
C ₅ H ₄ O ₂ S	2-thiophenecarboxylic acid						
400.9	21.0	0	52.4	41.3	21.0	16.6	[144]
	A14+2*A15+A131+2*A18+A18*B18+A19+A36*B36						
C ₅ H ₄ O ₂ S	3-thiophenecarboxylic acid						
412.9	18.3	0	44.32	39.9	18.3	16.5	[144]
	A14+2*A15+A131+A18+2*A18*B18+A19+A36*B36						
C ₅ H ₄ O ₃	2-furancarboxylic acid						
402.5	22.6	0	56.15	39.6	22.6	16.0	[244]
	A14+2*A15+A112+2*A18+A18*B18+A19+A36*B36						
C ₅ H ₄ O ₃	3-furancarboxylic acid						
394.8	21.3	0	53.95	38.2	21.3	15.1	[244]
	A14+2*A15+A112+A18+2*A18*B18+A19+A36*B36						
C ₅ H ₅ N ₃ O ₂	2-amino-5-nitropyridine						
461.4	29.2	0	63.29	57.2	29.2	26.4	[427]
	3*A10+2*A12+A45+A50+A41						
C ₅ H ₆ N ₂	glutaronitrile						
242.0	12.03	0	49.71	63.3	12.03	15.3	[402]
	2*A56+3*A2*B2						
C ₅ H ₆ O ₅	2-ketoglutaric acid						

	388.7	28.59	0	73.55	62.4	28.59	24.2
	2*A2+A36+A35+A36*B36						[329]
C ₅ H ₈ F ₄ N ₄ O ₂		4,4-bis(difluoroamino)-1-nitropiperidine					
	336.2	50.2	0	149.3	132.2	50.2	44.4
	+A14+3*A15+A120+A51+A17+4*A48+2*A43						[103]
C ₅ H ₈ N ₄ O ₆		1,4,4-trinitropiperidine					
	389.2	100.4	0	258.0	56.0 ^a	100.4	21.8
	A14+3*A15+A17+A120+2*A50+A51						[103]
C ₅ H ₈ O ₄		1,5-pentanedioic acid (glutaric acid)					
	338.0	2.4	7.10				
	371.0	23.0	61.99	69.1	60.3	25.4	22.4
	Independent values for another reference						
	340.5	2.3	6.75				
	363.9	18.8	51.66	58.4	60.3	21.1	22.0
	3*A2*B2+2*A36*B36						[45, 298]
C ₅ H ₁₀ N ₂ O ₂		glutaramide					
	453.9	38.4	0	84.6	83.7	38.4	38.0
	3*A2*B2+2*A61						[357]
C ₅ H ₁₀ O ₃		diethyl carbonate					
	198.2	9.24	0	46.6	42.3	9.24	8.4
	2*A1+2*A2+A149						[154]
C ₅ H ₁₁ NO		pentanamide					
	211.8	1.9	8.97				
	365.0	1.20	3.29				
	377.2	17.9	47.45	59.7	73.4	21.0	27.7
	A1+3*A2*B2+A61						[391]
C ₅ H ₁₁ NO		2,2-dimethylpropanamide					
	425.4	24.1	0	56.7	57.7	24.1	24.6
	3*A1+A4*B4+A61						[391]
C ₅ H ₁₂ N ₂ O		1-butyl urea					
	310.5	6.3	20.29				
	346.2	0.7	2.02				
	365.4	10.8	29.56	51.9	59.6	17.8	21.8
	3*A2*B2+A1+A67						[305]

C ₅ H ₁₂ O	1-pentanol						
195.6	10.51	0	53.7	56.5	10.5	11.1	
	A1+4*A2*B2+A30						[187]
C ₅ H ₁₂ O	2,2-dimethyl-1-propanol						
329.8	3.87	0	11.73	26.8	3.87	8.8	
	Independent values from another reference						
242.0	4.46	18.43					
325.0	4.06	12.49	30.9	26.8	8.52	8.7	
	Independent values from another reference						
233.3	4.1	17.57					
328.2	2.9	8.84	26.4	26.8	7.0	8.8	
	3*A1+A4+A2+A30						[218,219, 395]
C ₅ H ₁₂ O	1,1-dimethyl-1-propanol (<i>tert</i> -amyl alcohol)						
146	1.96	13.43					
213	0.17	0.79					
264	4.46	16.88	31.1	38.6	6.59	10.2	
	3*A1+A2+A4*B4+A30						[221]
	Note: Compound was incorrectly listed as 2,2-dimethyl-1-propanol in our first paper [198]						
C ₅ H ₁₂ O	2-methyl-2-butanol						
145.8	0.9	6.17					
264.7	2.0	7.55	13.7	38.6	2.9	10.2	
	3*A1+A4*B4+A2+A30						[395]
C ₅ H ₁₂ O ₅	xylitol						
369.0	33.26	0	90.1	96.0	33.26	35.4	
	2*A2+3*A3*B3+5*A30*D30						[429]
C ₅ H ₁₄ N ₂	pentane-1,5-diamine						
285.0	29.82	0	104.6	89.3	29.82	25.5	
	5*A2*B2+2*A45						[15]
C ₆ Br ₆	hexabromobenzene						
598.8	24.6	0	41.1	60.0	24.6	35.9	
	6*A12+6*A21						[203]
C ₆ N ₈ O ₈	4,4''-dinitro-3,3':4',3'''-ter-1,2,5-oxadiazole-2'-oxide						
381.9	93.83	0	245.7		93.83		

	prediction not made					[273]
C ₆ HBr ₅ O	pentabromophenol					
469.8	27.6	0	58.75	62.8	27.6	29.5
	6*A12+A31+5*A21					[300]
C ₆ H ₂ Br ₄	1,2,4,5-tetrabromobenzene					
454.5	24.4	0	53.7	54.8	24.4	24.9
	2*A10+4*A12+4*A21					[203]
C ₆ H ₂ N ₄	2,3-dicyanopyrazine					
405.1	19.8	0	48.9	57.0	19.8	23.1
	2*A10+2*A12+2*A41+2*A56					[359]
C ₆ H ₂ N ₄ O ₆	4,6-dinitrobenzofurazan 3-oxide					
452.7	20.73	0	45.8	54.8	20.73	24.8
	A14+2*A15+2*A19+2*A10+2*A12+A118+A123+2*A50					[95]
C ₆ H ₃ Br ₃	1,2,4-tribromobenzene					
317.0	17.9	0	56.5	52.2	17.9	16.5
	3*A10+3*A12+3*A21					[203]
C ₆ H ₃ Br ₃	1,3,5-tribromobenzene					
395.0	21.72	0	55.0	52.2	21.72	20.6
	3*A10+3*A12+3*A21					[280]
C ₆ H ₃ Br ₃ O	2,4,6-tribromophenol					
367.5	20.9	0	56.9	57.6	20.9	21.2
	4*A12+2*A10+3*A21+A31					[300]
C ₆ H ₃ Cl ₂ NO ₂	3,4-dichloronitrobenzene					
314.1	17.95	0	57.1	66.0	17.95	20.7
	3*A10+3*A12+3*A22*D22+A50					[147]
C ₆ H ₃ Cl ₃	1,3,5-trichlorobenzene					
335.9	17.56	0	52.3	48.3	17.56	16.2
	3*A10+3*A12+3*A22*D22					[280]
C ₆ H ₃ Cl ₄ N	2-chloro-5-(trichloromethyl)pyridine					
324.7	14.50	0	44.7	57.8	14.50	18.8
	10+A12+A11+A41+4*A22*D22+A4*B4					[276]

C ₆ H ₄ Br ₂	1,4-dibromobenzene						
	357.7	18.6	0	52.00	49.6	18.6	17.7
	Independent value from another reference						
	360.5	20.39	0	56.56	49.6	20.39	17.8
		4*A10+2*A12+2*A21					[203, 280]
C ₆ H ₄ Br ₃ N	2,4,6-tribromoaniline						
	393.0	25.75	0	65.5	58.7	25.75	23.1
		2*A10+4*A12+A45+3*A21					[371]
C ₆ H ₄ ClF	1-chloro-4-fluorobenzene						
	245.0	13.9	0	56.7	47.4	13.9	11.6
		4*A10+2*A12+A24+A22*D22					[261]
C ₆ H ₄ ClNO ₂	2-chloronitrobenzene						
	305.8	18.21	0	59.6	48.5	18.21	14.8
		Independent value from another reference					
	305.8	18.11	0	59.2	48.5	18.11	14.8
		4*A10+2*A12+A50+A22*D22					[147, 385]
C ₆ H ₄ ClNO ₂	3-chloronitrobenzene						
	318.0	18.65	0	58.7	48.5	18.65	15.4
		Independent value from another reference					
	316.9	19.52	0	61.6	48.5	19.52	15.4
		4*A10+2*A12+A50+A22*D22					[147, 385]
C ₆ H ₄ ClNO ₂	4-chloronitrobenzene						
	356.1	16.17	0	45.4	48.5	16.17	17.3
		Independent value from another reference					
	355.1	15.03	0	42.3	48.5	15.03	17.2
		4*A10+2*A12+A50+A22*D22					[147, 385]
C ₆ H ₄ ClNO ₃	2-chloro-4-nitrophenol						
	380.7	20.88	0	54.9	53.9	20.88	20.5
		3*A10+3*A12+A50+A31+A22*D22					[397]
C ₆ H ₄ ClNO ₃	4-chloro-2-nitrophenol						
	360.3	22.69	0	63.0	53.9	22.69	19.4
		3*A10+3*A12+A50+A31+A22*D22					[397]

C ₆ H ₄ ClNO ₃	4-chloro-3-nitrophenol						
399.4	25.97	0	65.0	53.9	25.97	21.5	
	3*A10+3*A12+A50+A31+A22*D22						[397]
C ₆ H ₄ Cl ₂	1,4-dichlorobenzene						
275.0	1.24	4.51					
306.0	0.18	0.59					
326.2	17.91	54.90	60.0	47.0	19.33	15.3	
	4*A10+2*A12+2*A22*D22						[280]
C ₆ H ₄ Cl ₂ N ₂ O ₂	2,6-dichloro-4-nitrobenzenamine						
467.2	29.48	0	63.1	56.3	29.48	26.3	
	2*A10+4*A12+2*A22*D22+A45+A50						[197]
	[Note: Compound was incorrectly listed in our earlier compilation [198] as 2,6-dichloro-4-benzenamine]						
C ₆ H ₄ N ₂ O ₄	1,3-dinitrobenzene						
360.4	19.68	0	54.6	50.0	19.68	18.0	
	4*A10+2*A12+2*A50						[157]
C ₆ H ₄ N ₂ O ₄	1,4-dinitrobenzene						
446.0	17.58	0	39.4	50.0	17.58	22.3	
	4*A10+2*A12+2*A50						[157]
C ₆ H ₄ N ₂ O ₅	2,3-dinitrophenol						
419.0	22.67	0	54.1	62.9	22.67	26.4	
	3*A10+2*A12+2*A50+A31						[157]
C ₆ H ₄ N ₂ O ₅	2,4-dinitrophenol						
383.2	26.19	0	68.4	62.9	26.19	24.1	
	3*A10+2*A12+2*A50+A31						[157]
C ₆ H ₄ N ₂ O ₅	2,6-dinitrophenol						
329.0	22.91	0	69.6	62.9	22.91	20.7	
	3*A10+2*A12+2*A50+A31						[157]
C ₆ H ₄ O ₂	1,4-benzoquinone						
385.1	18.40	0	47.8	29.4	18.40	11.3	
	3*A15+A14+4*A18*B18+2*A114						[202]
C ₆ H ₅ Br ₂ N	2,4-dibromoaniline						

	351.4	21.37	0	60.8	56.1	21.37	19.7
							[371]
	3*A10+3*A12+A45+2*A21						
C ₆ H ₅ Br ₂ N		2,5-dibromoaniline					
	328.1	20.47	0	62.4	56.1	20.47	18.4
							[371]
	3*A10+3*A12+A45+2*A21						
C ₆ H ₅ Br ₂ N		2,6-dibromoaniline					
	355.5	21.79	0	61.3	56.1	21.79	19.9
							[371]
	3*A10+3*A12+A45+2*A21						
C ₆ H ₅ BrO		4-bromophenol					
	338.2	17.6	0	52.0	52.4	17.6	17.7
							[300]
	A21+4*A10+2*A12+A31						
C ₆ H ₅ Cl ₂ N		3,4-dichloroaniline					
	344.5	21.69	0	63.0	53.5	21.69	18.4
							[147]
	3*A10+3*A12+A45+2*A22*D22						
C ₆ H ₅ NO ₂		nicotinic acid					
	509.3	97.10	0	190.7	49.2 ^a	97.1	25.1
	[Note: Compound is already in database – this value is considerably larger than previously reported value – it is likely in error]						
	Independent value from another source						
	451.4	0.81	1.79				
	509.1	27.57	54.15	55.9	49.2	28.38	25.1
							[269, 443]
	4*A10+A12+A41+A36*B36						
C ₆ H ₅ NO ₃		2-nitrophenol					
	316.3	17.05	0	53.9	52.6	17.05	16.6
							[157]
	4*A10+2*A12+A50+A31						
C ₆ H ₅ NO ₃		3-nitrophenol					
	369.0	18.06	0	48.94	52.6	18.06	19.4
							[157]
	4*A10+2*A12+A50+A31						
C ₆ H ₅ NO ₃		4-nitrophenol					
	386.4	11.00	0	28.47	52.6	11.00	20.3
							[157]
	4*A10+2*A12+A50+A31						
C ₆ H ₅ NO ₃		(2-furyl)oxoacetamide					

(I)	373.4	22.0	0	58.92	57.5	22.0	21.5
(II)	367.2	17.8	0	48.47	57.5	17.8	21.1
		A14+2*A15+A112+A18*B18+A19+A18+A35+A61					[433]
C ₆ H ₆ BrN		2-bromoaniline					
	304.1	16.14	0	53.08	53.5	16.14	16.3
		4*A10+2*A12+A45+A21					[371]
C ₆ H ₆ BrN		4-bromoaniline					
	336.0	16.75	0	49.85	53.5	16.75	18.0
		4*A10+2*A12+A45+A21					[371]
C ₆ H ₆ ClN		2-chloroaniline					
	269.2	12.38	0	45.99	52.2	12.38	14.1
		4*A10+2*A12+A45+A22*D22					[385]
C ₆ H ₆ ClN		4-chloroaniline					
	343.5	21.06	0	61.31	52.2	21.06	17.9
		Independent value from another reference					
	342.8	20.47	0	59.71	52.2	20.47	17.9
		4*A10+2*A12+A45+A22*D22					[147, 385]
C ₆ H ₆ IN		2-iodoaniline					
	329.6	19.38	0	58.80	55.4	19.38	18.3
		4*A10+2*A12+A45+A29					[358]
C ₆ H ₆ IN		4-iodoaniline					
	336.0	16.94	0	50.42	55.4	16.94	18.6
		4*A10+2*A12+A45+A29					[358]
C ₆ H ₆ N ₂ O		2-pyridinealdoxime					
	388.0	19.98	0	51.50	51.9	19.98	20.1
		4*A10+A12+A41+A53+A6					[404]
C ₆ H ₆ N ₂ O		nicotinamide					
	401.6	25.50	0	63.50	60.9	25.50	24.5
		4*A10+A12+A41+A61					[437]
C ₆ H ₆ N ₄ O ₄		(2,4-dinitrophenyl)hydrazine					
	474.1	18.89	0	39.84	51.2	18.89	28.3
		3*A10+3*A12+2*A50+A44+A45					[157]

$C_6H_6N_{12}O_{12}$	hexanitrohexaazaisowurtzitane						
428.2	1.97	4.60					
435.2	5.91	13.58		208.9 ^a		89.5	
	Independent value from another reference						
442.2	7.25	16.40		208.9 ^a		92.4	
	4*A14+3*A15+6*A120+6*A51						[309, 310]
	Note: Neither paper reported enthalpy of fusion						
C_6H_6OS	3-acetylthiophene						
333.6	18.9	0	56.7	45.9	18.9	15.3	
	A14+2*A15+2*A18*B18+A18+A19+A131+A1+A35						[347]
$C_6H_6O_2$	1,2-dihydroxybenzene						
377.6	22.87	0	60.6	55.2	22.9	20.8	
	4*A10+2*A31+2*A12						[425]
$C_6H_6O_2$	1,4-dihydroxybenzene						
445.1	27.2	0	61.2	55.2	27.2	24.6	
	4*A10+2*A31+2*A12						[425]
$C_6H_6O_2S$	2-thiopheneacetic acid						
337.4	14.0	0	41.5	48.4	14.0	16.3	
	A14+2*A15+A18*B18+2*A18+A19+A131+A2+A36*B36						[347]
$C_6H_6O_2S$	3-thiopheneacetic acid						
353.3	18.8	0	53.2	47.0	18.8	16.6	
	A14+2*A15+2*A18*B18+A18+A131+A19+A2+A36*B36						[347]
$C_6H_6O_3$	1,2,3-trihydroxybenzene						
405.6	25.9	0	63.86	60.6	25.9	24.6	
	3*A10+3*A12+3*A31						[174]
$C_6H_6O_3$	1,2,4-trihydroxybenzene						
413.2	28.8	0	69.70	60.6	28.8	25.0	
	3*A10+3*A12+3*A31						[174]
$C_6H_6O_3$	1,3,5-trihydroxybenzene						
491.8	34.5	0	70.15	60.6	34.5	29.8	
	3*A10+3*A12+3*A31						[174]

C ₆ H ₇ NO	2-aminophenol	443.2	31.4	0	70.8	56.3	31.4	25.0
		Independent value from another reference						
		447.6	21.72	0	48.5	56.3	21.7	25.2
		4*A10+2*A12+A31+A45 [48, 306, 307]						
C ₆ H ₇ NO	3-aminophenol	390.7	23.9	0	61.2	56.3	23.9	22.0
		Independent value from another reference						
		396.8	22.0	0	55.3	56.3	22.0	22.3
		4*A10+2*A12+A31+A45 [48, 306, 307]						
C ₆ H ₇ NO	4-aminophenol	455.2	23.8	0	52.3	56.3	23.8	25.6
		4*A10+2*A12+A31+A45 [48]						
C ₆ H ₇ NO	4-pyridinemethanol	325.2	11.78	0	36.22	55.7	11.78	18.1
		4*A10+A11+A30*B30+A41+A2 [318]						
C ₆ H ₇ NO ₂ S	benzenesulfonamide	425.8	25.2	0	59.11	54.7	25.17	23.3
		5*A10+A12+A96 [292]						
C ₆ H ₈ F ₈ N ₄	1,1,4,4-tetrakis(difluoroamino)cyclohexane	382.2	46.02	0	120.4	131.3	46.02	50.2
		A14+3*A15+2*A17+4*A48 [103]						
C ₆ H ₈ N ₂	adiponitrile	275.0	18.0	0	65.5	72.6	18.0	20.0
		4*A2*B2+2*A56 [402]						
C ₆ H ₈ N ₂ O ₂	1,4-diisocyanatobutane	231.2	20.8	0	89.79	83.4	20.8	19.3
		4*A2*B2+2*A58 [328]						
C ₆ H ₈ N ₂ O ₂ S	sulfanilamide	435.4	23.3	0	53.5	61.2	23.3	26.6
		4*A10+2*A12+A45+A96 [168]						
C ₆ H ₈ N ₄ O ₈	1,1,4,4-tetranitrocyclohexane							

489.2	108.8	0	222.4	46.1 ^a	108.8	22.6
A14+3*A15+2*A17+4*A50						[103]
Note: Experimental enthalpy is abnormally large – compound may be decomposing						
C ₆ H ₉ N ₃ O ₂	2-amino-4,6-dimethoxypyrimidine					
371.0	29.9	0	80.5	72.7	29.9	27.0
A10+3*A12+2*A41+2*A1+2*A32+A45						[178]
C ₆ H ₉ N ₃ O ₃	2,4,6-trimethoxy-1,3,5-triazine					
340.2	3.9	11.46				
395.2	18.1	45.80	57.26	77.1	22.0	30.5
3*A1+3*A32+3*A41+3*A12						[38, 191]
C ₆ H ₉ N ₃ O ₃	6-methoxy-3,5-dimethyl-tetrahydrotriazine-2,4-dione					
363.2	12.7	0	34.97	46.8	12.7	17.0
[Note: Compound rearranges shortly after melting]						
A14+3*A15+2*A125+A118+A19+3*A1+A32						[38, 182]
C ₆ H ₁₀ O ₄	1,6-hexanedioic acid (adipic acid)					
419.0	33.7	0	80.43	69.6	33.7	29.2
4*A2*B2+2*A36*B36						[298]
C ₆ H ₁₀ O ₆	D-galactono-1,4-lactone					
410.3	35.8	0	87.2	86.1	35.8	35.3
A14+2*A15+A115+4*A30*D30+A2+3*A16+A3*B3						[281]
C ₆ H ₁₀ O ₆	L-galactono-1,4-lactone					
409.8	36.0	0	87.80	86.1	36.0	35.3
A14+2*A15+A115+4*A30*D30+A2+3*A16+A3*B3						[281]
C ₆ H ₁₀ O ₆	D-gulono-1,4-lactone					
459.3	40.1	0	87.4	86.1	40.1	39.6
A14+2*A15+A115+4*A30*D30+A2+3*A16+A3*B3						[281]
C ₆ H ₁₀ O ₆	L-gulono-1,4-lactone					
459.0	41.5	0	90.4	86.1	41.5	35.5
A14+2*A15+A115+4*A30*D30+A2+3*A16+A3*B3						[281]
C ₆ H ₁₀ O ₆	L-mannono-1,4-lactone					
426.5	36.1	0	84.7	86.1	36.1	36.7
A14+2*A15+A115+4*A30*D30+A2+3*A16+A3*B3						[281]

C ₆ H ₁₁ NO	caprolactam						
342.2	16.2	0	47.2	50.9	16.2	17.4	
	A14+4*A15+A124						[393]
C ₆ H ₁₁ NO	cyclohexanone oxime						
362.5	12.7	0	35.03	45.8	12.7	16.6	
	Independent value from another reference						
362.2	12.45	0	34.37	45.8	12.45	16.6	
	A14+3*A15+A19+A53						[45, 375]
C ₆ H ₁₁ NO ₂	5,5-dimethylperhydro-1,3-oxazine-2-one						
399.0	28.5	0	71.4	60.4	28.5	24.1	
	2*A1+A14+3*A15+A17+A154						[60]
	[Note: Melting point temperature and entropy of fusion incorrectly given in our earlier compilation.]						
C ₆ H ₁₂ N ₂ OS	N,N,N',N'-tetramethylmonothiooxamide						
350.2	17.0	0	48.5	45.7	17.0	16.0	
	4*A1+A59+A175						[27]
C ₆ H ₁₂ N ₂ O ₂	N,N,N',N'-tetramethyloxamide						
352.2	18.0	0	51.11	48.0	18.0	16.9	
	4*A1+2*A59						[27]
C ₆ H ₁₂ N ₂ O ₂	adipamide						
458.4	1.59	3.47					
499.1	52.7	105.6	109.1	93.0	54.3	46.4	
	4*A2*B2+2*A61						[357]
C ₆ H ₁₂ N ₂ O ₄	2,3-dimethyl-2,3-dinitrobutane						
322.0	1.0	3.11					
389.0	18.0	46.27					
473.0	8.8	18.60	67.98	59.9	37.8	28.3	
	4*A1+2*A4*B4+2*A50						[246]
C ₆ H ₁₂ N ₂ S ₂	N,N,N',N'-tetramethyldithiooxamide						
409.2	21.0	0	51.32	43.4	21.0	17.8	
	4*A1+2*A175						[27]
C ₆ H ₁₂ O ₂	<i>cis</i> 1,2-cyclohexanediol						

373.2	20.3	0	54.31	51.2	20.27	19.1
Independent value from another reference						
360.4	19.9	55.2				
371.6	3.3	8.9	64.1	50.4	23.2	18.7
A14+3*A15+2*A30*B30+2*A16						[96, 170, 390]
C ₆ H ₁₂ O ₂	<i>trans</i> 1,2-cyclohexanediol					
375.7	16.4	0	43.6	50.4	16.4	18.9
Independent value from another reference						
382.6	21.0	0	54.89	50.4	21.0	19.3
A14+3*A15+2*A30*B30+2*A16						[96, 170, 390]
C ₆ H ₁₂ S ₃	1,4,7-trithiacyclononane					
354.2	29.0	0	81.9	64.3	29.0	22.8
A14+6*A15+3*A131						[1]
C ₆ H ₁₃ NO	hexanamide					
305.1	7.9	25.89				
373.0	16.7	44.77	70.66	82.7	24.6	30.8
A1+4*A2*B2+A61						[391]
C ₆ H ₁₄ N ₂	<i>trans</i> -cyclohexyl-1,4-diamine					
342.1	27.0	0	78.92	57.9	27.0	19.8
A14+3*A15+2*A45+2*A16						[383]
C ₆ H ₁₄ N ₂ O	1-pentyl urea					
355.1	2.5	7.04				
375.2	21.0	55.97	63.01	68.9	23.5	25.9
A1+A67+4*A2*B2						[305]
C ₆ H ₁₄ O	3,3-dimethyl-1-butanol					
235.7	9.54	0	40.5	33.9	9.54	8.0
3*A1+2*A2+A4+A30						[254]
C ₆ H ₁₄ O ₂	2,2-dimethoxybutane					
174.0	9.32	0	53.56	64.0	9.32	11.1
4*A1+A2+A4*B4+2*A32						[58]
C ₆ H ₁₄ O ₂	1,1-diethoxyethane					
167.0	10.95	0	65.6	66.6	11.0	11.1
3*A1+2*A2+A3*B3+2*A32						[58]

C ₆ H ₁₄ O ₂	1,6-hexanediol						
316.0	25.5	0	80.70	91.1	25.5	28.8	
	2*A30*B30+6*A2*B2						[321]
C ₆ H ₁₄ O ₃	2-ethyl-2-(hydroxymethyl)-1,3-propanediol						
327.8	16.4	49.9					
332.7	0.9	2.70	52.6	60.7	17.3	20.2	
	A1+4*A2+A4+3*A30*C30						[149]
C ₆ H ₁₄ O ₆	sorbitol						
369.2	30.35	0	82.20	108.5	30.35	40.0	
	2*A2+4*A3*B3+6*A30*D30						[435]
C ₆ H ₁₆ N ₂	hexane-1,6-diamine						
312.3	40.21	0	128.8	98.6	40.21	30.8	
	6*A2*B2+2*A45						[15]
C ₆ H ₁₈ AsN ₃	<i>tris</i> (dimethylamino)arsine						
222.6	13.3	0	59.79	42.1	13.31	9.4	
	6*A1+3*A43+A98						[12]
C ₇ H ₄ Cl ₂ O	2,4-dichlorobenzaldehyde						
347.2	20.47	0	59.0	53.6	20.5	18.6	
	3*A10+3*A12+A34+2*A22*D22						[185]
C ₇ H ₄ N ₂ O ₂	2-nitrobenzotrile						
338.1	1.57	4.64					
382.7	15.7	41.1	45.7	50.0	17.3	19.1	
	4*A10+2*A12+A50+A56						[14]
C ₇ H ₄ N ₂ O ₂	3-nitrobenzotrile						
389.7	20.49	0	52.6	50.0	20.5	19.5	
	4*A10+2*A12+A50+A56						[14]
C ₇ H ₄ N ₂ O ₂	4-nitrobenzotrile						
349.0	0.45	1.29					
386.0	1.01	2.62					
420.6	17.73	42.15	46.1	50.0	19.2	21.0	
	4*A10+2*A12+A50+A56						[14]

C ₇ H ₄ N ₂ O ₅	2,4-dinitrobenzaldehyde						
344.9	21.18	0	61.4	56.6	21.2	19.5	[267]
	3*A10+3*A12+A34+2*A50						
C ₇ H ₅ BrO ₂	2-bromobenzoic acid						
421.6	24.83	0	58.9	48.3	24.8	20.4	[265]
	4*A10+A36*B36+2*A12+A21						
C ₇ H ₅ BrO ₂	3-bromobenzoic acid						
430.1	24.91	0	57.9	48.3	24.9	20.8	[265]
	4*A10+A36*B36+2*A12+A21						
C ₇ H ₅ BrO ₂	4-bromobenzoic acid						
526.3	30.87	0	58.7	48.3	30.9	25.4	[265]
	4*A10+A36*B36+2*A12+A21						
C ₇ H ₅ ClO ₂	2-chlorobenzoic acid						
414.0	25.25	0	61.0	47.0	25.3	19.5	[265]
	4*A10+A36*B36+2*A12+A22*D22						
C ₇ H ₅ ClO ₂	3-chlorobenzoic acid						
427.9	23.67	0	55.32	47.0	23.7	20.1	[265]
	4*A10+A36*B36+2*A12+A22*D22						
C ₇ H ₅ ClO ₂	4-chlorobenzoic acid						
512.5	30.91	0	60.31	47.0	30.91	24.1	[265]
	4*A10+A36*B36+2*A12+A22*D22						
C ₇ H ₅ NOS	2-mercaptobenzoxazole						
470.0	25.0	0	53.19	48.4	25.0	22.7	
	Independent value from another reference						
468.3	22.56	0	48.17	48.4	22.56	22.7	[387, 407]
	A14+2*A15+4*A10+2*A19+A163						
C ₇ H ₅ NO ₃ S	1,1-dioxo-1,2-benzisothiazol-3(2H)-one (Saccharin)						
500.7	29.89	0	59.7	59.7	29.9	29.9	[292]
	4*A10+A14+2*A15+2*A19+A166						
C ₇ H ₅ NO ₄	5-nitro-1,3-benzodioxole						
420.2	28.20	0	67.1	51	28.2	21.4	[396]
	A14+2*A15+2*A112+2*A19+3*A10+A12+A50						

C ₇ H ₅ NS ₂	2-mercaptobenzothiazole						
455.9	22.3	0	48.9	48.4	22.3	22.1	
	Independent value from another source						
453.5	20.56	0	45.33	48.4	20.56	21.9	
	A14+2*A15+4*A10+2*A19+A163						[387, 407]
C ₇ H ₆ Cl ₂ O	2,3-dichloroanisole						
304.1	22.04	0	72.48	54.4	22.04	16.5	
	3*A10+3*A12+A1+A32+2*A22*D22						[408]
C ₇ H ₆ Cl ₂ O	3,5-dichloroanisole						
310.5	23.68	0	76.26	54.4	23.68	16.9	
	3*A10+3*A12+A1+A32+2*A22*D22						[408]
C ₇ H ₆ N ₂	benzimidazole						
384.4	0.71	1.85					
445.5	20.47	45.95	47.80	45.4	21.18	20.2	
	4*A10+A118+A121+A14+2*A15+2*A19+A18*B18						[9]
C ₇ H ₆ N ₂ S	2-mercaptobenzimidazole						
589.4	24.11	0	40.9	40.9	24.1	24.1	
	A14+2*A15+4*A10+2*A19+ A168						[407]
C ₇ H ₆ O ₂	4-hydroxybenzaldehyde						
390.8	21.6	0	55.4	56.4	21.6	22.0	
	4*A10+2*A12+A31+A34						[440]
C ₇ H ₆ O ₃	2-hydroxybenzoic acid						
432.4	26.1	0	60.4	51.1	26.1	22.1	
	Independent value from another reference						
431.1	24.45	0	56.7	51.1	24.5	22.0	
	4*A10+2*A12+A31+A36*B36						[327, 416]
C ₇ H ₆ O ₃	3-hydroxobenzoic acid						
476.4	36.5	0	76.62	51.1	36.5	24.4	
	4*A10+2*A12+A31+A36*B36						[327]
C ₇ H ₆ O ₃	4-hydroxybenzoic acid						
487.2	31.4	0	64.45	51.1	31.4	24.9	
	Independent value from another reference						

	489.0	30.85	0	63.1	51.1	30.85	25.0
							[2, 355]
$C_7H_6O_3$							
	337.7	16.96	0	50.22	53.6	16.96	18.1
							[177]
$C_7H_7ClN_2O_2$							
	323.4	19.5	0	60.3	58.7	19.5	19.0
							[127]
$C_7H_7NO_2$							
	411.9	29.0	0	70.41	62.8	29.0	25.9
							[365]
$C_7H_7NO_2$							
	445.7	33.7	0	75.61	52.2	33.7	23.3
							[48]
$C_7H_7NO_2$							
	459.2	24.5	0	53.35	52.2	24.5	24.0
	355.2	2.06	5.80				
	458.7	22.62	49.31	55.11	52.2	24.68	24.0
							[48, 294]
$C_7H_7NO_2$							
(I)	414.9	15.42	0	37.17	56.6 ^a	15.42	24.0
(II)	417.6	22.12	0	52.97	56.6	22.12	23.6
							[434]
$C_7H_7NO_3$							
	406.2	47.9	0	117.9	71.6	47.9	29.1
							[48]
$C_7H_7NO_3$							
	543.2	67.2	0	123.7	71.6	67.2	38.9
							[48]
$C_7H_7NO_4$							
	374.4	21.69	0	57.93	60.0	21.69	22.5

		3*A10+3*A12+A50+A31+A1+A32					[209]
C ₇ H ₇ NO ₄	2-methoxy-5-nitrophenol						
377.6	21.43	0	56.75	60.0	21.43	22.7	
		3*A10+3*A12+A50+A31+A1+A32					[209]
C ₇ H ₇ NO ₄	4-methoxy-2-nitrophenol						
352.3	22.42	0	63.64	60.0	22.42	21.1	
		3*A10+3*A12+A50+A31+A1+A32					[209]
C ₇ H ₇ N ₃ O ₄	N-methyl-N-(4-nitrophenyl)nitramine						
416.9	25.0	0	60.0	60.2	25.0	25.1	
		A1+4*A10+2*A12+A47+A51+A50					[127]
C ₇ H ₇ N ₃ O ₄	N-methyl-N-(3-nitrophenyl)nitramine						
350.5	25.3	0	72.18	60.2	25.3	21.1	
		A1+4*A10+2*A12+A47+A51+A50					[127]
C ₇ H ₈	bicyclo[2,2,1]-hepta-2,5-diene						
202.0	8.20	40.59					
255.6	1.91	7.47	48.1	34.7	10.1	8.9	
		2*A14+A15+4*A18+2*A16					[344]
C ₇ H ₈ O	2-methylphenol						
305.4	14.8	0	48.5	50.4	14.8	15.4	
		A31+A1+A12+4*A10+A11					[420]
C ₇ H ₈ O	3-methylphenol						
282.3	8.9	0	31.5	50.4	6.9	14.2	
		A31+A1+A12+4*A10+A11					[420]
C ₇ H ₈ O	4-methylphenol						
308.8	12.6	0	40.8	50.4	12.6	15.6	
		A31+A1+A12+4*A10+A11					[420]
C ₇ H ₈ O ₂	2-hydroxybenzyl alcohol						
358.3	21.5	0	60.0	57.6	21.5	20.6	
		4*A10+A31+A12+A11+A2+A30*B30					[436]
C ₇ H ₁₀ ClN ₃ O ₃	1-(2-hydroxy-3-chloropropyl)-2-methyl-5-nitroimidazole (Ornidazole)						
358.6	21.38	0	59.62	72.5	21.38	26.0	

A1+A14+2*A15+2*A2+A30*D30+A22*D22+A3*B3+A50+A18*B18+
2*A19+A118+A119 [176]

C₇H₁₀N₂ pimelonitrile
241.7 15.0 0 62.1 81.9 15.0 19.8
5*A2*B2+2*A56 [402]

C₇H₁₀N₂ 4-N,N-dimethylaminopyridine
387.1 21.63 0 55.9 46.0 21.63 17.8
2*A1+4*A10+A12+A41+A43 [374]

C₇H₁₂ norbornane
360.8 4.45 0 12.3 41.1 4.45 14.8
2*A14+A15+2*A16 [188]

C₇H₁₂O₂ cyclohexylcarboxylic acid
301.9 9.20 0 30.5 43.2 9.2 13.0
A14+3*A15+A16+A36 [377]

C₇H₁₂O₄ 1,7-heptanedioic acid (pimilic acid)
337.7 1.5 4.44
368.2 23.7 64.37 68.8 78.9 25.2 29.1
5*A2*B2+2*A36*B36
[298]

C₇H₁₄N₂O₂ pimelamide
446.8 44.56 0 99.73 102.3 44.6 45.7
5*A2*B2+2*A61 [357]

C₇H₁₄O cycloheptanol
227.9 0.45 1.97
250.4 0.78 3.12
278.3 1.51 5.43 10.5 35.2 2.7 9.8
A14+4*A15+A30+A16 [220]

C₇H₁₆N₂O 1-hexyl urea
383.0 22.4 0 58.49 78.2 22.4 30.0
A1+A67+5*A2*B2 [305]

C₇H₁₆O 1-heptanol
239.9 18.35 0 76.5 75.1 18.4 18.0

	A1+6*A2*B2+A30						[293]
C ₇ H ₁₆ O	propyl <i>tert</i> -butyl ether						
179.6	9.87	0	55.0	59.2	9.9	10.6	
	4*A1+A2+A4*B4+A32						[20, 308]
C ₇ H ₁₆ O	isopropyl <i>tert</i> -butyl ether						
184.8	8.46	0	45.78	59.9	8.46	11.1	
	5*A1+A4*B4+A32+A3*B3						[20, 308]
C ₇ H ₁₈ N ₂	heptane-1,7-diamine						
298.5	36.95	0	123.8	107.9	37.0	32.2	
	7*A2*B2+2*A45						[15]
C ₈ Cl ₄ N ₂	2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile						
423.7	4.03	9.51		55.2 ^a		23.4	
	Enthalpy of fusion not reported in paper						
	6*A12+4*A22*D22+2*A56						[315]
C ₈ H ₅ NO ₂	1 <i>H</i> -indole-2,3-dione (isatin)						
475.7	27.82	0	58.5	47.1	27.8	22.4	
	4*A10+A14+2*A15+2*A19+A114+A124						[169]
C ₈ H ₅ NO ₂	5-cyano-1,3-benzodioxole						
366.3	20.79	0	56.8	51.0	20.79	18.7	
	A14+2*A15+2*A19+2*A112+A56+3*A10+A12						[396]
C ₈ H ₅ NO ₃	2 <i>H</i> -1,3-benzoxazine-2,4(3 <i>H</i>)-dione						
500.5	28.63	0	57.20	55.3	28.63	27.7	
	A14+3*A15+A115+A124+2*A19+4*A10						[184]
C ₈ H ₆ ClN	2-(chloromethyl)benzonitrile						
334.2	20.53	0	61.43	53.5	20.53	17.9	
	4*A10+A12+A11+A2+A22*D22+A56						[386]
C ₈ H ₆ ClNS ₂	2-(chloromethylthio)benzothiazole						
351.1	17.02	0	54.04	62.3	17.02	21.9	
	4*A10+A14+2*A15+3*A19+A118+A131+A2+A84+A22*D22						[268]
C ₈ H ₆ Cl ₂ O ₃	2,4-dichlorophenoxyacetic acid						
416.2	32.0	0	76.9	69.4	32.0	28.9	

		3*A10+3*A12+A2+2*A22*D22+A36*D36+A32					[289]
C ₈ H ₆ F ₁₂ O ₄	3,3,4,4,6,6,7,7,9,9,10,10-dodecafluoro-2,5,8,11-tetraoxododecane						
239.0	22.07	92.34					
251.0	1.14	4.54	96.9	81.3	23.2		
	A14+11*A15+4*A112+6*A17+12*A28					[320]	
C ₈ H ₆ O ₃	4-formylbenzoic acid						
452.2	21.3	0	47.10	52.3	21.3	23.7	
	4*A10+2*A12+A36*B36+A34					[230]	
C ₈ H ₆ S ₂	2,2'-bithiophene						
304.2	16.5	0	54.2	50.3	16.5	15.3	
	2*A14+4*A15+2*A19+2*A18*B18+4*A18+2*A131					[347]	
C ₈ H ₆ O ₄	1,3-benzodioxole-5-carboxylic acid (piperonylic acid)						
501.6	30.50	0	60.81	56.1	30.5	28.1	
	A14+2*A15+2*A19+A12+2*A10+2*A112+A36*D36					[177]	
C ₈ H ₇ ClN ₂ O ₂	N-(2-chlorophenyl)-2-(hydroxyimino)acetamide						
432.7	29.7	0	68.64	49.9	29.7	21.6	
	4*A10+2*A12+A60+A6*B6+A53+A22*D22					[102]	
C ₈ H ₇ ClO ₂	2-chlorophenylacetic acid						
367.4	24.33	0	66.2	52.0	24.3	19.1	
	4*A10+A11+A12+A2+A22*D22+A36*B36					[413]	
C ₈ H ₇ ClO ₂	3-chlorophenylacetic acid						
349.8	22.60	0	64.61	52.0	22.0	18.2	
	4*A10+A11+A12+A2+A22*D22+A36*B36					[413]	
C ₈ H ₇ ClO ₂	4-chlorophenylacetic acid						
377.9	23.57	0	62.37	52.0	23.6	19.7	
	4*A10+A11+A12+A2+A22*D22+A36*B36					[413]	
C ₈ H ₈ BrNO	4-bromoacetanilide						
441.2	25.8	0	58.48	51.2	25.8	22.6	
	4*A10+2*A12+A1+A60+A21					[243]	
C ₈ H ₈ N ₂	2-methylbenzimidazole						
383.9	0.59	1.54					

	451.4	20.49	45.39	46.93	53.8	21.08	24.3	
		4*A10+A118+A121+A14+2*A15+3*A19+A1						[9]
C ₈ H ₈ N ₂ O ₂		2-(hydroxyimino)-N-phenylacetamide						
	453.1	10.4	0	23.0	48.6	10.4	22.0	
		5*A10+A12+A60+A6*B6+A53						[102]
C ₈ H ₈ O ₂		phenylacetic acid						
	349.2	15.2	0	43.5	47.9	15.2	16.7	
		5*A10+A11+A2+A36						[2]
C ₈ H ₈ O ₂		4'-hydroxyacetophenone						
	382.8	18.08	0	47.2	57.1	18.1	21.9	
		4*A10+2*A12+A31+A35+A1						[448]
C ₈ H ₈ O ₃		4-hydroxyphenylacetic acid						
	422.9	28.0	0	66.2	56.1	28.0	23.7	
		4*A10+A11+A12+A2+A36*B36+A31						[2]
C ₈ H ₈ O ₃		1,3-benzodioxole-5-methanol (piperonyl alcohol)						
	327.1	18.05	0	55.2	54.8	18.1	17.9	
		A14+2*A15+2*A19+2*A112+3*A10+A11+A2+A30*C30						[177]
C ₈ H ₈ O ₃		1-cyclohexene-1,2-dicarboxylic acid anhydride						
	343.5	11.88	0	34.6	55.6	11.9	19.1	
		2*A14+3*A15+A117+2*A19						[239]
C ₈ H ₈ O ₃		methyl 4-hydroxybenzoate						
	399.2	25.3	0	63.4	60.2	25.3	24.0	
		4*A10+2*A12+A1+A31+A38						[438]
C ₈ H ₈ O ₃		4-hydroxy-3-methoxybenzaldehyde (vanillin)						
	355.4	22.4	0	63.0	63.8	22.4	22.7	
		3*A10+3*A12+A31+A34+A1+A32						[440]
C ₈ H ₈ S		2,3-dihydrobenzo[b]thiophene						
	269.8	14.84	0	55.0	48.7	14.84	13.1	
		4*A10+A14+2*A15+2*A19+A131						[145]
C ₈ H ₉ ClN ₂ O		2-chloro-N,N-dimethylnicotinamide						
	342.2	21.39	0	62.51	76.4	21.39	26.1	

								3* A_{10} +2* A_{12} +2* A_1 + A_{41} + A_{62} + A_{22} * D_{22}	[334]
C_8H_9NO	acetanilide								
387.2	18.3	0	47.26	48.6	18.3	18.8			
	5* A_{10} + A_{12} + A_1 + A_{60}								[243]
$C_8H_9NO_2$	4-(acetylamino)phenol (acetaminophen)								
441.9	26.49	0	59.8	54.0	26.5	23.9			
	4* A_{10} + A_{60} + A_1 +2* A_{12} + A_{31}								[350]
$C_8H_9NO_2$	2-amino-3-methylbenzoic acid								
447.4	27.30	0	61.02	52.8	27.30	23.6			
	A_1 +3* A_{10} +2* A_{12} + A_{11} + A_{45} + A_{36} * B_{36}								[8]
$C_8H_9NO_2$	2-amino-5-methylbenzoic acid								
450.0	27.63	0	61.40	52.8	27.63	23.8			
	A_1 +3* A_{10} +2* A_{12} + A_{11} + A_{45} + A_{36} * B_{36}								[8]
$C_8H_9NO_2$	2-amino-6-methylbenzoic acid								
398.7	27.49	0	69.0	52.8	27.5	21.1			
	A_1 +3* A_{10} +2* A_{12} + A_{11} + A_{45} + A_{36} * B_{36}								[8]
$C_8H_9NO_2$	3-amino-2-methylbenzoic acid								
458.8	38.47	0	83.9	52.8	38.5	24.2			
	A_1 +3* A_{10} +2* A_{12} + A_{11} + A_{45} + A_{36} * B_{36}								[8]
$C_8H_9NO_2$	3-amino-4-methylbenzoic acid								
438.8	26.89	0	61.3	52.8	26.9	23.2			
	A_1 +3* A_{10} +2* A_{12} + A_{11} + A_{45} + A_{36} * B_{36}								[8]
$C_8H_9NO_2$	4-amino-3-methylbenzoic acid								
439.4	21.77	0	49.5	52.8	21.8	23.2			
	A_1 +3* A_{10} +2* A_{12} + A_{11} + A_{45} + A_{36} * B_{36}								[8]
$C_8H_9NO_2$	3-aminophenylacetic acid								
468.2	42.7	0	91.2	57.2	42.7	26.8			
	4* A_{10} + A_{11} + A_{12} + A_{45} + A_{36} * B_{36} + A_2								[2]
$C_8H_9NO_2S_2$	N-theonylthiocarbamic-O-ethyl ester								
345.9	21.90	0	63.3	54.6	21.9	18.9			
	A_{14} +2* A_{15} + A_{131} +2* A_{18} + A_{18} * B_{18} + A_{19} + A_{60} + A_{176} + A_1 + A_2								[403]

C ₈ H ₉ N ₃ O ₂	N-(1-oxopropyl)pyrazinecarboxamide						
366.7	23.5	0	64.09	71.6	23.5	26.3	
	3*A10+A12+2*A41+A2+A1+A71						[86]
C ₈ H ₁₀ Cl ₂ O ₂	3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylic acid						[55701-05-8]
331.5	16.32	0	49.2	61.8	16.3	20.5	
	A14+2*A1+A17+2*A16+2*A22*D22+A36*D36+A6+A7						[445]
C ₈ H ₁₀ N ₂ O ₃	N-methyl-N-(4-methoxyphenyl)nitramine						
342.6	22.7	0	66.3	64.8	22.7	22.2	
	4*A10+2*A12+2*A1+A32+A47+A51						[127]
C ₈ H ₁₀ N ₂ O ₃ S	sulfacetamide						
455.2	29.8	0	65.5	65.5	29.8	29.8	
	4*A10+2*A12+A1+A45+A173						[168]
C ₈ H ₁₀ N ₂ O ₄ S	N-methyl-N-(3-methylsulfonylphenyl)nitramine						
377.8	26.1	0	69.1	59.5	26.1	22.5	
	4*A10+2*A12+2*A1+A88+A47+A51						[127]
C ₈ H ₁₀ N ₂ O ₄ S	N-methyl-N-(4-methylsulfonylphenyl)nitramine						
438.1	19.2	0	43.8	59.5	19.2	26.1	
	4*A10+2*A12+2*A1+A88+A47+A51						[127]
C ₈ H ₁₀ N ₄ O ₂	caffeine						
428.2	4.02	9.39					
510.2	21.9	42.92	52.3	40.8	25.9	20.8	
	Independent value from another reference						
420.9	3.43	8.15					
509.5	19.86	38.98	47.1	40.7	23.4	20.8	
	2*A14+3*A15+2*A125+3*A1+2*A19+A18*B18+A119+A118						[363, 405]
C ₈ H ₁₀ O	4-methylbenzyl alcohol						
179.0	0.73	4.08					
210.0	0.21	1.00					
331.9	20.17	60.77	65.85	43.9	21.11	14.57	
	A1+2*A2+4*A10+2*A11+A30						[340]
C ₈ H ₁₀ O ₃	1,2-cyclohexanedicarboxylic anhydride						
303.8	14.71	0	48.42	50.8	14.71	15.4	

		2*A14+3*A15+2*A16+A117					[442]
C ₈ H ₁₁ N ₃ O ₄	methyl N-(4,6-dimethoxypyrimidin-2-yl)carbamate						
357.2	26.29	0	73.6	83.2	26.3	29.4	
	3*A1+A10+A12+2*A41+A69						[278]
C ₈ H ₁₂ N ₂	suberonitrile						
268.9	21.97	0	81.70	91.2	21.97	24.5	
	6*A2*B2+2*A56						[402]
C ₈ H ₁₂ OS	2-oxa-6-thiaadamantane						
224.0	4.11	18.35					
557.0	8.12	14.56	32.91	49.2	12.23	27.4	
	3*A14+A15+4*A16+A112+A131						[26]
C ₈ H ₁₂ O ₂	2,6-dioxadamantane						
276.0	5.84	21.16					
444.0	3.78	8.51	29.7	47.5	9.6	21.1	
	3*A14+A15+4*A16+2*A112						[26]
C ₈ H ₁₂ S ₆	1,3,5,7-tetramethyl-2,4,6,8,9,10-hexathiatricyclo[3.3.1.1 ^{3,7}]decane						
501.4	23.7	0	47.27	53.3	23.7	26.7	
	3*A14+A15+6*A131+4*A1+4*A17						[150]
C ₈ H ₁₄ O ₂	cyclohexylacetic acid						
302.6	13.80	0	45.60	43.2	13.80	13.1	
	A14+3*A15+A36+A16						[377]
C ₈ H ₁₄ O ₄	1,8-octanedioic acid (suberic acid)						
335.9	2.0	5.95					
403.6	9.1	22.55					
413.2	30.7	74.30	102.8	88.2	41.8	36.5	
	6*A2*B2+2*A36*B36						[298]
C ₈ H ₁₅ N ₅ S	Simetryn						
353.2	24.0	0	68.0	68.7	24.0	24.3	
	3*A12+3*A41+2*A44+A84+3*A1+2*A2						[392]
C ₈ H ₁₅ N ₇ O ₂ S ₂	N ⁷ (aminosulfonyl)-3-[[2-(diaminomethyleneamino)-4-thiazoyl]methylthio]-propanamidine (Famotidine)						
(I) 444.4	45.81	0	103.1		45.8		

(II)	436.6	43.92	0	100.6		43.9		[23]
		prediction not made						
C ₈ H ₁₆		ethylcyclohexane						
	161.5	8.5	0	52.6	54.5	8.5	8.80	[368]
		A14+A16+A1+A2+3*A15						
C ₈ H ₁₆ N ₂ O ₂		suberamide						
	431.3	5.45	12.64					
	493.2	58.4	118.4	131.0	111.6	63.9	55.0	[357]
		6*A2*B2+2*A61						
C ₈ H ₁₆ O		cyclooctanol						
	264.1	2.05	7.76					
	297.1	1.97	6.63	14.39	38.9	4.02	11.6	[220]
		A14+5*A15+A16+A30						
C ₈ H ₁₆ S ₄		1,4,7,10-tetrathiacyclododecanone						
	499.2	31.0	0	62.10	67.2	31.0	33.5	[1]
		A14+6*A15+4*A131						
C ₈ H ₁₇ NO		octanamide						
	194.4	1.91	9.83					
	304.5	0.97	3.19					
	377.0	27.6	73.21	86.23	101.3	30.48	38.2	[391]
		A1+6*A2*B2+A61						
C ₈ H ₁₈ N ₂ O		1-heptyl urea						
	386.1	29.0	0	75.1	87.5	29.0	33.8	[305]
		A1+A67+6*A2*B2						
C ₈ H ₁₈ O		1-octanol						
	258.4	25.24	0	97.7	84.4	25.2	21.8	[293]
		A1+7*A2*B2+A30						
C ₈ H ₁₈ O		isobutyl <i>tert</i> -butyl ether						
	162.3	8.65	0	53.3	48.6	8.7	7.9	[332]
		5*A1+A32+A4+A3+A2						
C ₈ H ₁₈ O ₂		2,2,4-trimethyl-1,3-pentanediol						
	328.3	24.2	0	73.7	51.8	24.2	17.0	

							4*A1+A2+A3*B3+A3+A4+2*A30*B30	[301]
C ₈ H ₁₉ NSi	triethylsilylethyleneimine	183.6	14.25	0	77.6	61.1	14.3	11.2
							+A14+A119+A109+3*A1+3*A2	[21]
C ₈ H ₂₀ N ₂	octane-1,8-diamine	324.8	50.98	0	157.0	117.2	51.0	38.1
							8*A2*B2+2*A45	[15]
C ₉ H ₆ N ₂ O ₃	5-nitro-8-quinolinol	453.2	24.7	0	54.5	55.9	24.7	25.3
							5*A10+4*A12+A41+A31+A50	[33]
C ₉ H ₆ O ₂	1,3-indandione	401.5	21.8	0	54.3	43.0	21.8	17.3
							A14+2*A15+2*A19+2*A114+4*A10	[388]
C ₉ H ₇ BrO ₂	3-bromo- <i>trans</i> -cinnamic acid	443.2	31.06	0	70.1	56.3	31.1	24.9
							4*A10+2*A12+A21+A36*B36+2*A6*B6	[71]
C ₉ H ₇ NO	8-quinolinol	346.8	22.1	0	63.7	53.1	22.1	18.4
							6*A10+3*A12+A41+A31	[33]
C ₉ H ₇ NO ₂	1-methyl-1 <i>H</i> -indole-2,3-dione (N-methylisatin)	403.3	19.50	0	48.4	40.3	19.5	16.3
							A1+4*A10+A14+2*A15+2*A19+A114+A125	[169]
C ₉ H ₈ Cl ₂ O ₃	2-(2,4-dichlorophenoxy)propionic acid	391.3	32.0	0	81.78	74.7	32.0	29.2
							3*A10+3*A12+2*A22*D22+A36*D36+A32+A1+A3*B3	[289]
C ₉ H ₈ Cl ₂ O ₃	2,4-dichlorophenoxyacetic acid, methyl ester	313.4	20.0	0	63.82	69.2	20.0	21.7
							3*A10+3*A12+A2+A1+A32+A38+2*A22*D22	[289]
C ₉ H ₈ O	1-indanone	314.1	17.6	0	56.03	48.1	17.6	15.1
							4*A10+A14+3*A15+2*A19+A114	[388]

C ₉ H ₈ O	2-indanone	330.0	16.89	0	50.7	48.1	16.9	15.9
			4*A10+A14+3*A15+2*A19+A114					[388]
C ₉ H ₈ O ₂	<i>trans</i> -cinnamic acid	406.1	22.21	0	54.7	52.2	22.2	21.2
			5*A10+A12+A6+A36+A6*B6					[416]
C ₉ H ₈ O ₃	5-oxoethyl-1,3-benzodioxole	358.9	26.23	0	73.17	55.5	26.2	19.9
			A14+2*A15+2*A19+2*A112+3*A10+A12+A1+A35					[396]
C ₉ H ₈ O ₄	acetylsalicylic acid (aspirin)	412.7	31.01	0	75.1	56.1	31.0	23.2
			Independent value from another reference					
		409.2	29.17	0	71.3	56.1	29.2	23.0
			A1+A38+A36*B38+4*A10+2*A12					[138, 139, 217]
C ₉ H ₈ O ₄	1,3-benzodioxole-5-acetic acid (homopiperonylic acid)	401.7	24.94	0	73.4	68.5	24.9	27.5
			+A14+2*A15+2*A19+2*A112+3*A10+A11+A2+A36*D36					[177]
C ₉ H ₈ O ₄	monomethyl phthalate	357.5	21.63	0	60.5	56.1	21.6	20.1
			4*A10+2*A12+A1+A38+A36*B36					[330]
C ₉ H ₈ O ₄	monomethyl isophthalate	466.7	36.50	0	78.2	56.1	36.5	26.2
			4*A10+2*A12+A1+A38+A36*B36					[330]
C ₉ H ₈ O ₄	monomethyl terephthalate	492.5	37.68	0	76.5	56.1	37.7	27.6
			4*A10+2*A12+A1+A38+A36*B36					[330]
C ₉ H ₉ N ₃ O ₂ S ₂	sulfathiazole	473.0	30.3	0	64.1	68.4	30.3	32.3
			A14+2*A15+4*A10+2*A12+A45+A95+2*A18*B18+A19+A118+A131					[168]
C ₉ H ₁₀ N ₂	N-(2-cyanoethyl)aniline	310.6	0.98	3.16				

	323.3	19.4	60.01	63.17	65.8	20.38	21.3
							[287]
	4*A10+A11+A12+2*A2+A45+A56						
C ₉ H ₁₀ N ₂ O ₃							
	457.6	8.3	0	18.14	56.0	8.3	25.6
							[102]
	4*A10+2*A12+A1+A32+A60+A6*B6+A53						
C ₉ H ₁₀ N ₂ O ₃							
	424.6	27.8	0	65.47	56.0	27.8	23.8
							[102]
	4*A10+2*A12+A1+A32+A60+A6*B6+A53						
C ₉ H ₁₀ N ₂ O ₃							
	N-(4-methyl-2-nitrophenyl)acetamide						
	White crystals						
	366.2	24.25	0	66.22	52.0	24.25	19.0
	Amber crystals						
	356.7	20.97	0	58.79	52.0	20.97	18.5
	Yellow crystals						
	364.2	22.37	0	61.42	52.0	22.37	18.9
							[24]
	2*A1+3*A10+2*A12+A11+A50+A60						
C ₉ H ₁₀ O ₃							
	349.8	23.1	0	66.0	70.9	23.1	24.8
							[440]
	3*A10+3*A12+A31+A34+A1+A32+A2						
C ₉ H ₁₀ O ₃							
	335.5	17.67	0	52.7	54.5	17.7	18.3
							[302]
	2*A14+3*A15+A1+A18+A19+2*A16+A117						
C ₉ H ₁₀ O ₃							
	317.0	20.3	0	64.1	65.8	20.3	20.9
							[440]
	3*A10+3*A12+2*A1+2*A32+A34						
C ₉ H ₁₀ O ₃							
	362.4	28.78	0	79.4	64.2	28.8	23.3
							[414]
	A14+3*A15+2*A19+4*A10+A16+A2+A30*D30						
C ₉ H ₁₀ O ₃							
	388.9	32.49	0	83.5	67.3	32.5	26.2
	Independent value from another source						
	389.0	26.4	0	67.9	67.3	26.4	26.2
							[437, 438]
	4*A10+2*A12+A1+A31+A38*B38+A2						

C ₉ H ₁₁ ClN ₂ O	N,N-dimethyl-N'-(4-chlorophenyl)urea (Monuron)	447.6	29.3	0	65.5	66.0	29.3	29.5	
								[210]	
			2*A1+A64 +A22*D22+2*A12+4*A10						
C ₉ H ₁₁ NO	2-(acetylamino)toluene	382.7	21.70	0	56.70	49.2	21.70	18.8	
								[306, 307]	
			2*A1+4*A10+A11+A12+A60						
C ₉ H ₁₁ NO	4-(acetylamino)toluene	424.0	28.93	0	68.23	49.2	28.93	20.9	
								[306, 307]	
			2*A1+4*A10+A11+A12+A60						
C ₉ H ₁₁ NO ₂ S ₂	N-theonylthiocarbamic-O-propyl ester	370.1	26.10	0	70.52	61.7	26.1	22.8	
								[403]	
			A14+2*A15+A131+2*A18+A18*B18+A19+A176+A1+2*A2						
C ₉ H ₁₂ N ₂ S	2-propyl-4-pyridinecarbothioamide	414.1	23.21	0	56.05	62.8	23.2	26.0	
								[444]	
			3*A10+A11+A12+A41+A92+A1+2*A2						
C ₉ H ₁₂	trispiro[2.0.2.0.2.0]nonane ([3] rotane)	312.1	14.14	0	45.3	18.7	14.1	5.8	
								[190]	
			4*A14-3*A15+3*A17						
C ₉ H ₁₂ O ₄	3,4,5-trimethoxyphenol	420.2	31.94	0	76.0	72.0	31.9	30.3	
								[410]	
			3*A1+A31+3*A32+2*A10+4*A12						
C ₉ H ₁₄ N ₂	azelanitrile	251.1	18.68	0	74.4	100.5	18.7	25.2	
								[402]	
			7*A2*B2+2*A56						
C ₉ H ₁₄ O	2-oxadamantane	567.0	8.12	0	14.3	46.3	8.1	26.3	
								[26]	
			3*A14+A15+4*A16+A112						
C ₉ H ₁₄ S	2-thiaadamantane	211.0	1.95	9.24					
		597.0	8.10	14.0	22.81	48.0	10.1	27.8	
								[26]	
			3*A14+A15+4*A16+A131						

C ₉ H ₁₆ O ₄	1,9-nonanedioic acid (azelaic acid)						
330.6	0.01	0.03					
339.8	0.7	2.06					
372.4	29.7	79.75	81.84	97.5	30.41	36.3	
	2*A36*B36+7*A2*B2						[298]
C ₉ H ₁₇ N ₅ S	Ametryn						
359.1	26.0	0	72.4	69.4	26.0	24.9	
	3*A12+3*A41+2*A44+A84+4*A1+A2+A3*B3						[392]
C ₉ H ₁₈	propylcyclohexane						
178.0	10.6	0	59.6	61.6	10.6	11.0	
	A14+A16+A1+2*A2+3*A15						[368]
C ₉ H ₁₈ N ₂ O ₂	azelamide						
450.4	55.0	0	122.11	120.9	55.0	54.5	
	7*A2*B2+2*A61						[357]
C ₉ H ₁₈ S ₄	1,5,9-trithiacyclododecane						
349.2	12.0	34.36					
373.2	19.4	51.98	86.3	75.4	31.4	28.1	
	A14+9*A15+3*A131						[1]
C ₉ H ₂₀ N ₂ O	1-octyl urea						
353.2	11.8	33.41					
374.6	24.4	65.14	98.6	96.8	36.2	36.3	
	A1+A67+7*A2*B2						[305]
C ₉ H ₂₀ O ₂	2-butyl-2-ethyl-1,3-propanediol						
317.3	20.8	0	65.6	78.3	20.8	24.8	
	2*A1+6*A2+A4+2*A30*B30						[301]
C ₉ H ₂₀ O ₂ S ₂	<i>meso</i> 1,3-bis(propylsufinyl)propane						
411.3	40.58	0	98.7	100.9	40.6	41.5	
	2*A1+7*A2+2*A87						[119]
C ₉ H ₂₀ O ₂ S ₂	<i>racemic</i> 1,3-bis(propylsufinyl)propane						
387.8	35.15	0	90.64	100.9	35.15	39.1	
	2*A1+7*A2+2*A87						[119]

C ₉ H ₂₁ As	tripropylarsine						
180.0	14.60	0	81.11	95.8	14.60	17.7	
	3*A1+6*A2+A98						[13]
C ₉ H ₂₂ N ₂	nonane-1,9-diamine						
301.7	7.77	25.75					
308.1	36.24	117.6	143.4	126.5	44.0	39.0	
	9*A2*B2+2*A45						[15]
C ₁₀ HCl ₇	1,2,3,4,5,6,7-heptafluoronaphthalene						
454.5	8.54	18.79					
456.0	8.75	19.19	38.0	56.1	17.3	25.6	
	A10+9*A12+7*A24						[356]
C ₁₀ H ₂ Cl ₆	1,2,4,5,6,8-hexachloronaphthalene						
449.4	28.89	0	64.3	52.0	28.9	23.4	
	2*A10+8*A12+6*A24						[356]
C ₁₀ H ₃ Cl ₅	1,2,3,5,7-pentachloronaphthalene						
444.9	27.14	0	61.0	50.7	27.1	22.6	
	3*A10+7*A12+5*A22*D22						[356]
C ₁₀ H ₃ Cl ₅	1,2,3,5,8-pentachloronaphthalene						
387.8	14.39	37.11					
443.4	0.92	2.07					
453.3	8.44	18.62	57.8	50.7	23.8	23.0	
	3*A10+7*A12+5*A22*D22						[356]
C ₁₀ H ₃ Cl ₅	1,2,3,6,7-pentachloronaphthalene						
416.6	22.94	0	55.1	50.7	22.9	21.1	
	3*A10+7*A12+5*A22*D22						[356]
C ₁₀ H ₃ Cl ₅	1,2,3,7,8-pentachloronaphthalene						
381.6	17.55	0	46.0	50.7	17.6	19.3	
	3*A10+7*A12+5*A22*D22						[356]
C ₁₀ H ₃ Cl ₅	1,2,4,5,6-pentachloronaphthalene						
404.2	15.64	38.69					
412.7	8.41	20.38	59.1	50.7	24.1	20.9	
	3*A10+7*A12+5*A22*D22						[356]

C ₁₀ H ₃ Cl ₅	1,2,4,6,7-pentachloronaphthalene	404.3	22.58	0	55.9	50.7	22.6	20.5
								[356]
			3*A10+7*A12+5*A22*D22					
C ₁₀ H ₃ Cl ₅	1,2,4,6,8-pentachloronaphthalene	429.0	19.75	0	46.0	50.7	19.8	21.8
								[356]
			3*A10+7*A12+5*A22*D22					
C ₁₀ H ₄ Cl ₄	1,2,3,4-tetrachloronaphthalene	440.5	10.53	23.90				
		454.3	1.33	2.93				
		470.8	11.54	24.51	51.34	49.4	23.4	23.3
								[356]
			4*A10+6*A12+4*A22*D22					
C ₁₀ H ₄ Cl ₄	1,2,7,8-tetrachloronaphthalene	401.3	14.62	0	36.43	49.4	14.6	19.8
								[356]
			4*A10+6*A12+4*A22*D22					
C ₁₀ H ₄ Cl ₄	1,3,5,7-tetrachloronaphthalene	453.0	27.14	0	59.91	49.4	27.1	22.4
								[356]
			4*A10+6*A12+4*A22*D22					
C ₁₀ H ₅ Cl ₃	1,2,3-trichloronaphthalene	354.7	18.44	0	51.99	48.1	18.4	17.1
								[356]
			5*A10+5*A12+3*A22*D22					
C ₁₀ H ₆ F ₃ NO ₂	4-trifluoromethyl-7-aminocoumarin	494.8	31.7	0	64.1	62.1	31.7	30.7
								[118]
			A14+3*A15+3*A10+A12+A45+A115+A18+3*A19+3*A25+A4*B4					
C ₁₀ H ₈	naphthalene	353.4	16.44	0	46.5	44.2	16.4	15.6
								[439]
			8*A10+2*A12					
C ₁₀ H ₉ N	2-methylquinoline	270.5	12.52	0	46.3	48.3	12.5	13.1
								[291]
			A1+6*A10+2*A12+A11+A41					
C ₁₀ H ₉ N	8-methylquinoline	246.9	10.73	0	43.46	48.3	10.7	11.9
								[291]
			A1+6*A10+2*A12+A11+A41					

C ₁₀ H ₁₀	pentacyclo[4.4.0.0 ^{2,5} .0 ^{3,8} .0 ^{4,7}]dec-9-ene (basketene)	331.8	2.72	0	8.20	31.4	2.7	10.4
								[171]
	5*A14-4*A15+8*A16+2*A18							
C ₁₀ H ₁₀	tricyclo[4.2.2.0 ^{2,5}]dec-3,7,9-triene	293.7	1.46	0	4.97	35.5	1.5	10.4
								[171]
	3*A14+A15+4*A16+6*A18							
C ₁₀ H ₁₀	2,2a,2b,3,5a,5b-hexahydro-1,2,3-metheno-1 <i>H</i> -cycloprop[cd]indene (snoutene)	334.0	7.87	0	23.56	74.0	7.87	24.7
								[171]
	4*A14-2*A15+6*A16+2*18							
C ₁₀ H ₁₀	1,2-dihydronaphthalene	264.4	10.53	0	39.8	46.3	10.5	12.2
								[409]
	A14+3*A15+2*A18+2*A19+4*A10							
C ₁₀ H ₁₀ Cl ₂ O ₃	4-(2,4-dichlorophenoxy)butanoic acid	395.5	35.0	0	88.50	86.2	35.0	34.1
								[289]
	3*A10+2*A12+A11+3*A2+2*A22*D22+A36*D36+A32							
C ₁₀ H ₁₀ N ₂	1,8-diaminonaphthalene	339.8	16.15	0	47.5	57.2	16.2	19.4
								[398]
	6*A10+4*A12+2*A45							
C ₁₀ H ₁₀ N ₄ O ₂ S	sulfadiazine	532.7	44.3	0	83.2	79.1	44.3	42.1
								[168]
	7*A10+3*A12+2*A41+A95+A45							
C ₁₀ H ₁₀ O ₂	<i>trans</i> methyl cinnamate	309.0	33.1	0	107.1	64.1	33.1	19.8
								[39]
	A1+5*A10+A12+A38+A6+A6*B6							
C ₁₀ H ₁₀ O ₂	4-methoxycinnamaldehyde	332.7	19.0	0	57.2	69.0	19.0	23.0
								[440]
	4*A10+2*A12+A1+A32+A34+2*A6							
C ₁₀ H ₁₀ O ₃	2-methoxycinnamic acid	458.7	32.54	0	70.9	62.4	32.5	28.6
								[111]
	4*A10+2*A12+A6+A36*B36+A6*B6+A1+A32							

C ₁₀ H ₁₀ O ₃	3-methoxycinnamic acid						
390.5	22.58	0	57.8	62.4	22.6	24.4	
	4*A10+2*A12+A6+A36*B36+A6*B6+A1+A32						[111]
C ₁₀ H ₁₀ O ₃	4-methoxycinnamic acid						
446.4	24.75	55.44					
461.9	2.49	5.39	60.8	62.4	27.2	28.9	
	4*A10+2*A12+A6+A36*B36+A6*B6+A1+A32						[111]
C ₁₀ H ₁₀ O ₄	4-hydroxy-3-methoxycinnamic acid						
435.3	17.89	0	41.1	81.7	17.9	35.6	
	3*A10+3*A12+A6+A36*D36+A6*B6+A1+A32+A31						[111]
C ₁₀ H ₁₀ O ₄	ferulic acid						
444.6	33.34	0	75.0	81.7	33.3	36.3	
	3*A10+3*A12+A6+A6*B6+A36*D36+A31+A32+A1						[416]
C ₁₀ H ₁₀ O ₄	(RS)-phenylsuccinic acid						
440.1	37.37	0	84.9	57.1	37.4	25.1	
	5*A10+A11+A2+2*A36*B36+A3*B3						[367]
C ₁₀ H ₁₀ O ₄	(S)-phenylsuccinic acid						
446.9	41.84	0	93.6	57.1	41.8	25.5	
	5*A10+A11+A2+2*A36*B36+A3*B3						[367]
C ₁₀ H ₁₁ N ₃ O ₃ S	sulfamethoxazole						
440.7	33.8	0	76.7	76.5	33.8	33.7	
	4*A10+2*A12+A14+2*A15+A1+A45+A95+A118+A112+A18+2*A19						[168]
C ₁₀ H ₁₂ N ₂	2-propylbenzimidazole						
385.8	1.5	3.89					
431.6	Not reported in paper			68.0 ^a		29.3	
	4*A10+A14+2*A15+3*A19+A118+A121+A1+2*A2						[207]
	Note: Authors did not report enthalpy of fusion data						
C ₁₀ H ₁₂ N ₂	2-isopropylbenzimidazole						
410.4	1.0	2.44					
507.9	Not reported in paper			55.0 ^a		34.5	
	4*A10+A14+2*A15+3*A19+A118+A121+2*A1+A3						[207]
	Note: Authors did not report enthalpy of fusion data						

C ₁₀ H ₁₂ N ₂ O ₃	N-(4-ethoxyphenyl)-2-(hydroxyimino)acetamide	491.2	7.6	0	15.5	63.1	7.6	31.0
								[102]
	4*A10+2*A12+A1+A32+A60+A6*B6+A53+A2							
C ₁₀ H ₁₂ N ₂ O ₃	N-(2-ethoxyphenyl)-2-(hydroxyimino)acetamide	424.6	27.8	0	65.5	63.1	27.8	26.8
								[102]
	4*A10+2*A12+A1+A32+A60+A6*B6+A53+A2							
C ₁₀ H ₁₂ N ₂ O ₄	(2-hydroxyethyl)[3-[(hydroxyimino)methyl]phenyl carbamic acid	508.3	28.9	0	56.9	56.9	28.9	28.9
								[102]
	3*A10+2*A12+A11+2*A2+A6*B6+A53+A30*C30+A178							
C ₁₀ H ₁₂ O ₂	2,3,5,6-tetramethyl-1,4-benzoquinone	384.1	18.39	0	47.9	62.9	18.4	24.2
								[202]
	4*A1+A14+3*A15+4*A19+2*A114							
C ₁₀ H ₁₂ O ₂	2-isopropyl-5-methyl-1,4-benzoquinone (thymoquinone)	323.2	18.16	0	56.2	47.4	18.2	15.3
								[232]
	3*A1+A14+3*A15+2*A19+2*A18*B18+2*A114+A3							
C ₁₀ H ₁₂ O ₃	propyl 4-hydroxybenzoate	369.3	27.2	0	73.7	74.4	27.2	27.5
								[438]
	4*A10+2*A12+A1+A31+A38*B38+2*A2							
C ₁₀ H ₁₂ O ₅	2,4,5-trimethoxybenzoic acid	417.9	31.15	0	74.5	81.9	31.2	34.2
								[306, 307]
	3*A1+2*A10+4*A12+3*A32+A36*D36							
C ₁₀ H ₁₂ O ₅	3,4,5-trimethoxybenzoic acid	444.5	29.90	0	67.3	81.9	29.9	36.4
								[306, 307]
	3*A1+2*A10+4*A12+3*A32+A36*D36							
C ₁₀ H ₁₃ NO ₂	4-ethoxyacetanilide	410.2	21.4	0	52.2	63.1	21.4	25.9
								[243]
	2*A1+4*A10+2*A12+A32+A60+A2							
C ₁₀ H ₁₃ NO ₂ S ₂	N-theonylthiocarbamic-O-butyl ester	364.3	23.89	0	65.6	68.8	23.9	25.1
								[403]
	A14+2*A15+A131+2*A18+A18*B18+A19+A60+A176+A1+3*A2							
C ₁₀ H ₁₃ N ₅ O ₄	3'-azido-2,3'-dideoxythymidine							

	395.8	33.03	0	83.45	78.0	33.0	30.9
	2*A14+5*A15+A112+A125+A124+A18*B18+A19+A1+A2+A30*D30+A46+3*A16						[148]
C ₁₀ H ₁₄ N ₄ O ₃	(R,S)-3,7-dihydro-7-(2-hydroxypropyl)-1,3-dimethyl-1 <i>H</i> -pyrine-2,6-dione (Proxiphylline)						
(I)	408.2	24.7	0	60.51	65.2	24.7	26.6
(II)	389.2	20.8	0	53.44	65.2	20.8	25.4
	2*A14+3*A15+3*A1+A2+2*A19+A18*B18+A118+A119+A3*B3+A30*D30+2*A119						[68]
C ₁₀ H ₁₅ Br	1-bromoadamantane						
	31.0	0.001	0.03				
	282.2	1.39	4.93				
	309.9	7.42	23.94				
	391.8	3.97	10.13	39.0	42.7	12.8	16.7
	3*A14+A15+3*A16+A17+A21						[270]
C ₁₀ H ₁₅ Cl	1-chloroadamantane						
	439.7	5.53	0	12.58	36.0 ^a	5.53	15.8
	3*A14+A15+3*A16+A17+A22						[42]
	[Note: Lower temperature transition was not reported. Compound is already in database.]						
C ₁₀ H ₁₅ N ₅ O ₃	9-(4-hydroxy-3-hydroxymethylbut-1-yl)guanine (Penciclovir)						[39809-25-1]
	551.2	35.74	0	64.84		35.74	
	prediction not made						[212]
C ₁₀ H ₁₆	<i>exo</i> tetrahydrodicyclopentadiene						
	162.1	3.18	19.62				
	183.2	1.20	6.55	26.17	45.1	4.32	8.3
	3*A14+A15+4*A16						[29]
C ₁₀ H ₁₆	<i>endo</i> tetrahydrodicyclopentadiene						
	213.8	10.7	50.04				
	356.8	3.48	9.75	59.79	45.1	14.18	16.1
	3*A14+A15+4*A16						[29]
C ₁₀ H ₁₆	<i>endo</i> tricyclo[5.2.1.0 ^(2,6)]decane						
	204.3	2.57	12.58				
	345.3	3.07	8.89	21.47	45.1	5.64	15.6

		3*A14+A15+4*A16					[162]	
C ₁₀ H ₁₆ N ₂	sebaconitrile							
		281.2	28.2	0	100.28	109.8	28.2	
			8*A2*B2+2*A56					30.9
							[402]	
C ₁₀ H ₁₆ O	1-adamantanol							
		357.1	11.29	31.62				
		552.9	12.36	22.35	54.0	26.9	23.7	
			3*A14+A15+3*A16+A17+A30					14.9
							[131]	
C ₁₀ H ₁₆ O	2-adamantanol							
		238.4	0.16	0.67				
		322.3	2.30	7.14				
		389.3	7.98	20.50				
		567.3	11.94	21.05	46.8	46.8	22.4	
			3*A14+A15+4*A16+A30					26.6
							[131]	
C ₁₀ H ₁₆ O ₂	chrysanthemic acid							
		390.7	14.51	0	37.1	47.8	14.5	
			A14+4*A1+A17+2*A16+A7+A6+A36					18.7
							[231]	
C ₁₀ H ₁₇ N	1-aminoadamantane							
		241.4	1.72	7.13				
		284.6	5.31	18.66		46.6 ^a	13.3	
			Note: Enthalpy of fusion not measured					
			3*A14+A15+3*A16+A17+A45					[412]
C ₁₀ H ₁₇ N ₅ O ₃	9-(4-hydroxy-3-hydroxymethylbut-1-yl)quinine							
		551.2	35.74	0	64.84		35.74	
			Structure not estimated					[212]
C ₁₀ H ₁₈	bicyclopentyl							
		171.5	0.26	1.52				
		237.8	13.40	56.35	57.87	52.2	13.66	
			2*A14+4*A15+2*A16					12.4
							[226]	
C ₁₀ H ₁₈ O ₄	1,10-decanedioic acid (sebacic acid)							
		370.3	0.4	1.08				
		403.9	46.6	115.38	115.5	106.8	47.0	
			Independent value from another reference					43.2

405.6	45.3	0	111.7	106.8	45.3	43.3
Independent value from another reference						
405.7	46.9	0	115.6	106.8	46.9	43.3
8*A2*B2+2*A36*B36 [298, 417, 431]						
C ₁₀ H ₁₉ N ₅ S	terbutryn					
376.1	21.0	0	55.8	73.8	21.0	27.8
5*A1+A2+A4*B4+2*A44+3*A41+3*A12+A84 [392]						
C ₁₀ H ₂₀	butylcyclohexane					
198.0	14.2	0	71.7	68.7	14.2	13.6
A14+A1+A16+3*A2+3*A15 [368]						
C ₁₀ H ₂₀	cyclodecane					
282.7	18.95	0	67.0	59.3	19.0	16.8
A14+7*A15 [312]						
C ₁₀ H ₂₀ N ₂ O ₂	N,N,N',N'-tetraethyloxamide					
310.2	17.0	0	54.8	76.4	17.0	23.7
4*A1+4*A2+2*A59 [27]						
C ₁₀ H ₂₀ N ₂ O ₂	sebacamide					
484.3	68.7	0	141.9	130.2	68.7	63.1
8*A2*B2+2*A61 [357]						
C ₁₀ H ₂₀ S ₄	1,4,8,11-tetrathiacyclotetradecane					
345.2	2.7	7.82				
393.2	33.0	83.93	91.8	85.7	35.7	33.7
A14+11*A15+4*A131 [1]						
C ₁₀ H ₂₀ S ₅	1,4,7,10,13-pentathiacyclopentadecane					
318.2	11.0	34.57				
340.2	4.2	12.35				
391.2	17.0	43.46	90.4	92.3	32.2	36.1
A14+12*A15+5*A131 [1]						
C ₁₀ H ₂₁ NO	decanamide					
218.7	1.05	4.80				
366.3	18.8	51.32				
370.6	15.1	40.74	96.9	119.9	35.0	44.4
A1+8*A2*B2+A61 [391]						

$C_{10}H_{22}N_2O$	1-nonyl urea						
380.3	38.9	0	102.3	106.1	38.9	40.4	
	A1+A67+8*A2*B2						[305]
$C_{10}H_{22}O$	1-decanol						
280.0	33.67	0	120.3	103.0	33.7	28.8	
	A1+9*A2*B2+A30						[293]
$C_{10}H_{22}Te$	dipentyl telluride						
215.4	23.1	0	107.2	114.7	23.1	24.7	
	2*A1+8*A2*B2+A140						[62]
$C_{10}H_{24}N_2$	decane-1,10-diamine						
332.9	57.81	0	173.7	135.8	57.81	45.2	
	10*A2*B2+2*A45						[15]
$C_{10}H_{27}N_5O_6$	8-[[[(1R)-1-(3,4-dimethoxyphenyl)-2-hydroxyethyl]amino]-3,7-dihydro-7-(2-methoxyethyl)-1,3-dimethyl-1H-pyridine-2,6-dione						[114606-56-3]
(I) 384.2	40.31	0	104.9	148	40.31	56.9	
(II) 401.2	39.88	0	99.40	148	39.88	59.4	
(III) 391.2	38.58	0	98.62	148	38.58	57.9	
	2*A14+3*A15+4*A1+3*A2+3*A19+A118+A119+3*A32+3*A10+2*A12+A11+A44+A30*D30+ 2*A124						[66]
$C_{11}H_8CrO_3$	styrenetricarbonyl chromium						
354.4	25.28	0	71.3	72.9	25.28	25.8	
	5*A10+A12+A5+A6+A189						[167]
$C_{11}H_{10}N_2O$	2-(2-benzofuryl) Δ -2-imidazoline						
(I) 412.7	25.95	0	62.9	64.3	26.0	26.5	
(II) 420.3	28.53	0	67.9	64.3	28.5	27.0	
	2*A14+4*A15+A118+A121+A112+4*A19+A18+4*A10						[74]
$C_{11}H_{11}N_3O_2S$	sulfapyridine						
462.7	40.47	0	87.5	75.6	40.47	35.0	
	8*A10+3*A12+A41+A45+A95						[168]
$C_{11}H_{12}Cl_2O_3$	4-(2,4-dichlorophenoxy)butanoic acid, methyl ester						
309.7	22.0	0	71.04	81.3	22.0	25.2	
	3*A10+2*A12+A11+2*A22*D22+A32+3*A2+A1+A38						[289]

$C_{11}H_{12}N_2OS_2$	2-(4-morpholinothio)benzothiazole							
(I)	345.0	12.97	0	37.6	65.4	13.0	25.2	
(II)	357.0	17.99	0	50.4	65.4	18.0	22.6	
		$2*A_{14}+5*A_{15}+A_{112}+A_{119}+A_{131}+A_{118}+3*A_{19}+4*A_{10}+A_{84}$						[84]
$C_{11}H_{12}N_4O_2S$	Sulfamerazine							
	508.5	41.3	0	81.2	79.7	41.3	40.5	
		$6*A_{10}+3*A_{12}+A_{11}+A_1+2*A_{41}+A_{95}+A_{45}$						[168]
$C_{11}H_{14}O_3$	butyl 4-hydroxybenzoate							
	341.8	26.6	0	77.8	81.5	26.6	27.9	
		$4*A_{10}+2*A_{12}+A_1+A_{31}+A_{38}*B_{38}+3*A_2$						[438]
$C_{11}H_{15}NO_2$	4-aminobenzoic acid, butyl ester							
	330.6	23.9	0	72.3	82.6	23.9	27.3	
		$4*A_{10}+2*A_{12}+3*A_2+A_1+A_{38}+A_{45}$						[335]
$C_{11}H_{15}NO_2$	4-aminobenzoic acid, 2-methylpropyl ester							
	327.8	10.7	0	32.64	69.6	10.7	22.8	
		$4*A_{10}+2*A_{12}+A_2+2*A_1+A_3+A_{38}+A_{45}$						[335]
$C_{11}H_{15}NO_2S_2$	N-theonylthiocarbamic-O-pentyl ester							
	354.3	24.59	0	69.40	75.9	24.6	26.9	
		$A_{14}+2*A_{15}+A_{131}+2*A_{18}+A_{18}*B_{18}+A_{19}+A_{176}+A_1+4*A_2$						[403]
$C_{11}H_{15}N_3O_2$	N-caproylpyrazinamide							
	351.7	35.95	0	102.2	92.9	35.95	32.7	
		$3*A_{10}+A_{12}+2*A_{41}+4*A_2+A_1+A_{71}$						[86]
$C_{11}H_{16}N_2O_2$	N-methyl-N-(4- <i>tert</i> -butylphenyl)nitramine							
	351.2	23.4	0	66.63	58.4	23.4	20.5	
		$4*A_1+A_4+4*A_{10}+A_{11}+A_{12}+A_{47}+A_{51}$						[127]
$C_{11}H_{18}N_2$	undecanedinitrile							
	266.1	26.0	0	97.71	119.1	26.0	31.7	
		$9*A_2*B_2+2*A_{56}$						[402]
$C_{11}H_{22}N_2O_2$	undecandiamide							
	451.2	64.4	0	142.7	139.5	64.4	62.9	
		$9*A_2*B_2+2*A_{61}$						[357]

C ₁₁ H ₂₀ O ₄	1,11-undecanedioic acid						
355.3	1.6	4.50					
380.1	41.2	108.39	112.9	116.1	42.8	44.1	
	9*A2*B2+2*A36*B36						[298]
C ₁₁ H ₂₄ N ₂ O	1-decyl urea						
294.4	1.3	4.42					
385.3	38.3	99.40	103.8	115.4	39.6	44.5	
	A1+A67+9*A2*B2						[305]
C ₁₁ H ₂₆ N ₂	undecane-1,11-diamine						
313.6	48.08	0	153.3	145.1	48.1	45.5	
	11*A2*B2+2*A45						[15]
C ₁₂ F ₂₃ N	perfluoro-N-(4-methylcyclohexyl)piperidine						
293.3	8.32	0	28.37	56	8.32	16.4	
	2*A14+6*A15+11*A17+19*A28+A119+3*A25+A4*B4+A28						[381]
C ₁₂ H ₈ N ₂	1,10-phenanthroline						
391.1	11.8	0	30.2	51.0	11.8	19.9	
	8*A10+4*A12+2*A41						[426]
C ₁₂ H ₈ O	dibenzofuran						
355.1	19.41	0	54.7	52.0	19.4	18.5	
	A14+2*A15+A112+2*A19+8*A10+2*A19						[439]
C ₁₂ H ₈ OS	phenoxathiin						
329.6	19.43	0	59.0	58.6	19.4	19.3	
	3*A15+A14+4*A19+8*A10+A131+A112						[389]
C ₁₂ H ₈ O ₂ S	dibenzothiophene 5,5'-dioxide						
509.2	27.17	0	53.4	48.6	27.2	24.7	
	A14+2*A15+4*A19+A134+8*A10						[382]
C ₁₂ H ₉ Cl ₂ NO ₃ S	N-(2,3-dichlorophenyl)benzenesulfonamide						
387.2	27.2	0	70.3	68.2	27.2	26.4	
	8*A10+4*A12+2*A22*D22+A95						[373]
C ₁₂ H ₉ F ₃ N ₂ O ₂	Leflunomide						
438.2	32.43	0	74.0	63.4	32.4	27.8	

C ₁₂ H ₁₁ N ₃ S	N-2-pyridyl-N'-phenylthiourea						
????	41.0	0		58.2 ^a	41.0		
	9*A10+3*A12+A41+A90						[6]
C ₁₂ H ₁₁ O ₂ P	P,P-diphenylphosphinic acid						
466.1	21.91	0	47.0	47.0	21.9	21.9	
	prediction not made						[376]
C ₁₂ H ₁₂	1,6-dimethylnaphthalene						
257.0	8.50	0	33.08	45.4	8.50	11.7	
	2*A1+2*A11+6*A10+2*A12						[394]
C ₁₂ H ₁₂	1,4-dimethylnaphthalene						
279.2	10.60	0	37.97	45.4	10.60	12.7	
	2*A1+2*A11+6*A10+2*A12						[394]
C ₁₂ H ₁₂	1,8-dimethylnaphthalene						
338.2	18.53	0	54.79	45.4	18.53	15.3	
	2*A1+2*A11+6*A10+2*A12						[394]
C ₁₂ H ₁₂	1,5-dimethylnaphthalene						
355.2	20.0	0	56.31	45.4	20.0	16.1	
	2*A1+2*A11+6*A10+2*A12						[394]
C ₁₂ H ₁₂	2,7-dimethylnaphthalene						
370.2	22.20	0	59.97	45.4	22.20	16.8	
	2*A1+2*A11+6*A10+2*A12						[394]
C ₁₂ H ₁₂	2,3-dimethylnaphthalene						
377.2	23.97	0	63.55	45.4	23.97	17.1	
	2*A1+2*A11+6*A10+2*A12						[394]
C ₁₂ H ₁₂	2,6-dimethylnaphthalene						
385.2	25.30	0	65.68	45.4	25.30	17.5	
	2*A1+2*A11+6*A10+2*A12						[394]
C ₁₂ H ₁₂ ClN ₅	2-amino-4-(<i>p</i> -chloranilino)-6-isopropenyl-S-triazine						
(I) 415.2	23.85	0	57.4	81.3	23.9	33.8	
(II) 403.2	20.50	0	50.8	81.3	20.5	32.8	
	4*A10+5*A12+3*A41+A44+A45+A22*D22+A1+A7+A5						[120]

C ₁₂ H ₁₂ N ₂ O ₃	Nalidixic acid	501.9	35.92	0	71.6	72.4	35.9	36.3
	A14+3*A15+3*A19+2*A10+A11+2*A1+A2+A41+A114+A119+A18*B18+A36*D36							[259]
C ₁₂ H ₁₂ O ₄	dimethyl 1,4-cubanedicarboxylate	438.2	38.1	0	87.0	34.3	38.1	15.0
	5*A14-7*A15+6*A16+2*A1+2*A38+2*A17							[319]
C ₁₂ H ₁₂ N ₂ O ₃	dimethyl 2,6-cuneanedicarboxylate	392.7	23.4	0	59.6	34.3	23.4	13.5
	5*A14-7*A15+6*A16+2*A1+2*A38+2*A17							[319]
C ₁₂ H ₁₂ S	1,2,3,4-tetrahydrodibenzothiophene	275.0	32.03	0	116.5	61.2	32.0	16.8
	4*A10+2*A14+3*A15+4*A19+A131							[206]
C ₁₂ H ₁₃ NO ₂ S	5,6-dihydro-2-methyl-N-phenyl-1,4-oxathin-3-carboxanilide (Carboxin)	365.3	28.19	0	77.2	72.6	28.2	26.5
	5*A10+A12+A14+3*A15+A1+A60+A112+A131+2*A19							[160]
C ₁₂ H ₁₃ N ₃	4,6-dimethyl-N-phenyl-2-pyrimidinamine	370.8	21.23	0	57.25	61.9	21.23	23.0
	6*A10+2*A12+2*A11+2*A41+2*A1+A44							[205]
C ₁₂ H ₁₄ Fe	ethyl ferrocene	273.9	12.29	0	44.9	61.4	12.3	16.8
	2*A14+4*A15+9*A18*B18+A180+A1+A2+A19							[121]
C ₁₂ H ₁₄ N ₄ O ₂ S	Sulfamethazine	469.0	39.2	0	83.6	80.3	39.2	37.7
	5*A10+3*A12+2*A11+2*A1+2*A41+A95+A45							[168]
C ₁₂ H ₁₅ N ₃ O ₆	5-tert-butyl-2,4,6-trinitro-1,3-dimethylbenzene (musk xylene)	386.7	20.79	0	53.8	55.0	20.8	21.3
	5*A1+3*A12+3*A11+3*A50+A4							[234]
C ₁₂ H ₁₆	tetraspiro[2.0.2.0.2.0.2.0]dodecane ([4] rotane)	394.9	21.00	0	53.2	17.5	21.00	6.9
	5*A14-3*A15+4*A17							[190]

C ₁₂ H ₁₆ N ₂ OS	N-[(3-methoxyphenyl)methyl]-N'-2-propenylthiourea					
313.0	15.43	0	49.3	79.4	15.4	24.9
	A90+2*A2+A5+A6+4*A10+A11+A12+A1+A32					[262]
C ₁₂ H ₁₆ N ₂ O ₄	2,4-dinitro-1,3-dimethyl-5- <i>tert</i> -butylbenzene					
340.4	16.68	0	49.0	52.2	16.7	17.8
	5*A1+A10+2*A12+3*A11+2*A50+A4					[234]
C ₁₂ H ₁₇ NO ₂ S ₂	N-theonylthiocarbamic-O-hexyl ester					
346.4	22.48	0	65.0	83.0	22.5	28.8
	A14+2*A15+A131+2*A18+A18*B18+A19+A176+A1+5*A2					[403]
C ₁₂ H ₁₈ ClNO	2-chloro- α -[[[(1,1-dimethylethyl)amino]methyl]benzenemethanol (Tulobuterol)					
(I) 364.0	27.1	0	74.5	67.0	27.1	24.4
(II) 354.0	25.4	0	71.8	67.0	25.4	23.7
	4*A10+A11+A12+3*A1+A4*B4+A3*B3+A2+A44+A30*C30+A22*D22					[283]
C ₁₂ H ₁₈ N ₂ O	N'-(<i>p</i> -cumenyl)-N,N-dimethylurea (Isoproturon)					
427.4	21.33	0	49.9	66.5	21.3	28.4
	4*A10+A12+A11+A3+A64+4*A1					[179]
C ₁₂ H ₂₀	1-ethyladamantane					
225.6	11.28	0	50.0	49.9	11.28	11.3
	3*A14+A15+3*A16+A17+A2+A1					[266]
C ₁₂ H ₂₀	1,3-dimethyladamantane					
223.4	9.31	41.67				
247.8	1.54	6.21	47.9	40.5	10.9	10.0
	3*A14+A15+2*A16+2*A17+2*A1					[266]
C ₁₂ H ₂₀ N ₂	dodecanedinitrile					
294.2	34.33	0	116.7	128.4	34.3	37.8
	10*A2*B2+2*A56					[402]
C ₁₂ H ₂₀ N ₂ O ₂	(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl diazoacetate					[63254-50-2]
320.4	17.20	0	53.7	53.7	17.2	17.2
	3*A1+A3+A14+3*A15+3*A16+A38+A178					[69]
C ₁₂ H ₂₀ O ₂	2-(1'-hydroxycyclohexyl)cyclohexanone					

	306.8	20.81	0	67.8	56.0	20.8	17.2
	2*A14+6*A15+A114+A17+A16+A30*B30						[338]
C ₁₂ H ₂₀ Si	tetraallylsilane						
	244.0	25.50	0	104.5	91.7	25.5	22.4
	4*A5+4*A2+4*A6+A109						[186]
C ₁₂ H ₂₂ O ₄	1,12-dodecanedioic acid						
	400.3	49.8	0	124.4	125.4	49.8	50.2
	Independent value from another reference						
	401.6	52.5	0	130.7	125.5	52.5	50.4
	10*A2*B2+2*A36*B36						[298, 431]
C ₁₂ H ₂₂ S	dicyclohexyl sulfide						
	274.7	10.01	36.44				
	284.2	5.68	19.99	56.4	61.7	15.7	17.5
	2*A14+6*A15+2*A16+A84						[166]
C ₁₂ H ₂₄ N ₂ O ₂	dodecandiamide						
	422.8	5.09	12.04				
	466.1	73.7	158.12	170.2	148.8	78.8	69.4
	10*A2*B2+2*A61						[357]
C ₁₂ H ₂₄ O ₁₁	1,4-O- α -D-glucopyranosyl-D-glucitol (maltitol)						
	420.0	55.07	0	131.1	159.3	55.1	66.9
	A14+3*A15+3*A2+9*A30*D30+A32+4*A3*B3+5*A16+A112						[37, 165]
C ₁₂ H ₂₄ S ₄	1,4,8,11-tetrathiacyclohexadecane						
(I)	328.2	32.0	97.50				
	333.2	5.2	15.61	113.1	93.1	37.2	31.0
(II)	328.2	27.0	82.27				
	333.2	5.2	15.61	97.9	93.1	32.2	31.0
	A14+13*A15+4*A131						[1]
C ₁₂ H ₂₅ NO	dodecanamide						
	321.1	9.7	30.21				
	373.3	36.3	97.24	127.5	138.5	46.0	51.7
	A1+10*A2*B2+A61						[391]
C ₁₂ H ₂₆ N ₂ O	1-undecyl urea						
	385.6	38.4	0	99.6	124.7	38.4	48.1

	A1+A67+10*A2*B2						[305]
C ₁₂ H ₂₆ O ₂	1,12-dodecanediol						
352.0	51.2	0	145.5	146.9	51.2	51.7	
	12*A2*B2+2*A30*B30						[399]
C ₁₂ H ₂₈ N ₂	dodecane-1,12-diamine						
340.5	67.10	0	197.1	154.4	67.1	52.6	
	12*A2*B2+2*A45						[15]
C ₁₃ H ₈ Cl ₂ O	4,4'-dichlorobenzophenone						
187.0	0.04	0.21					
192.0	0.05	0.26		81.2 ^a		15.2	
	Enthalpy of fusion and melting point temperature were not reported in paper						
	8*A10+2*A12+A35+2*A22*D22						[158]
C ₁₃ H ₈ Cl ₂ N ₂ O ₄	5-chloro-N-(2-chloro-4-nitrophenyl)-2-hydroxybenzamide (Niclosamide)						
502.2	35.98	0	71.6	71.3	36.0	35.8	
	Independent value from another reference						
505.4	40.7	0	80.5	71.3	40.7	36.0	
	6*A10+6*A12+A31+A50+2*A22*D22+A60						[213, 336]
C ₁₃ H ₈ F ₂ O ₃	5-[2,4-difluorophenyl]salicylic acid (Diflunisal)						
(I) 486.0	35.9	0	73.9	83.1	35.9	40.4	
(II) 485.5	35.8	0	73.7	83.1	35.8	40.3	
(III) 486.4	35.9	0	73.8	83.1	35.9	40.4	
	6*A10+6*A12+2*A24+A31+A36*D36						[88]
C ₁₃ H ₉ NO	9(10 <i>H</i>)-acridinone						
640.0	32.5	0	50.8	55.3	32.5	35.4	
	8*A10+A14+3*A15+4*A19+A121+A114						[180]
C ₁₃ H ₁₀ BrN ₃ O ₄	2-cyano-6-nitro-1(2 <i>H</i>)-quinolinecarboxylic acid, 2-bromoethyl ester						
419.2	19.79	0	47.2	61.6	19.8	25.8	
	A14+3*A15+3*A10+A12+2*A19+2*A18+A16+A50+A56+2*A2+A21+A179						[274]
C ₁₃ H ₁₀ ClN ₃ O ₄	2-cyano-6-nitro-1(2 <i>H</i>)-quinolinecarboxylic acid, 2-chloroethyl ester						
418.9	17.17	0	41.0	60.3	17.2	25.3	
	A14+3*A15+3*A10+A12+2*A19+2*A18+A16+A50+A56+2*A2+A22*D22+A169						[274]

C ₁₃ H ₁₀ N ₂ O ₄	Thalidomide						
	548.2	36.02	0	65.7	64.8	36.0	35.5
	Independent value from another source						
(I)	546.7	39.97	0	73.1	64.8	40.0	35.4
(II)	550.8	37.91	0	68.8	64.8	37.9	35.7
	4*A10+2*A14+5*A15+2*A19+A128+A129+A16 [73, 449]						
C ₁₃ H ₁₀ O	xanthene						
	374.6	20.67	0	55.2	55.7	20.7	20.9
	A14+3*A15+2*A19+8*A10+A112+2*A19 [389]						
C ₁₃ H ₁₀ O ₃	phenyl salicylate (salol)						
	315.0	19.16	0	60.8	72.1	19.2	22.7
	Independent value from another reference						
	314.2	18.98	0	60.4	72.1	19.0	22.6
	Independent values from another reference						
(I)	304.2	16.5	0	54.24	72.1	16.5	21.9
(II)	315.2	18.6	0	59.01	72.1	18.6	22.7
	Independent values from another reference						
	312.7	18.4	0	58.8	72.1	18.4	22.55
	9*A10+3*A12+A38+A31 [30, 279, 200, 370]						
C ₁₃ H ₁₀ O ₃	2,2'-dihydroxybenzophenone						
	334.5	20.07	0	60.0	74.4	20.1	24.9
	8*A10+4*A12+2*A31+A35 [325]						
C ₁₃ H ₁₁ BrO ₅	8-(hydroxymethyl)-6-bromo-2-oxo-2 <i>H</i> -1-benzopyran-3-carboxylic acid, ethyl ester						
	434.1	28.19	0	64.9	110.7	28.2	48.0
	A14+3*A15+A115+A18+A19+2*A10+A11+A12+2*A2+A30*D30+A21+A38+A1 [129]						
C ₁₃ H ₁₁ ClO ₅	8-(hydroxymethyl)-6-chloro-2-oxo-2 <i>H</i> -1-benzopyran-3-carboxylic acid, ethyl ester						
	418.2	15.53	37.14				
	424.0	22.47	53.00	90.1	109.4	38.0	46.4
	A14+3*A15+A115+A18+A19+2*A10+A11+A12+2*A2+A30*D30+A22*D22+A38+A1 [129]						
C ₁₃ H ₁₁ NO ₅	oxolinic acid						
	592.5	43.59	0	73.6	72.1	43.6	42.7
	2*A14+5*A15+5*A19+2*A112+A114+A119+A18*B18+A36*D36+A1+A2+2*A10 [260]						

C ₁₃ H ₁₁ N ₃ O ₂ S	5-methyl-2-[(4-methyl-2-nitrophenyl)amino]-3-thiophene carbonitrile	400.2	24.57	0	61.4	68.1	24.6	27.3
	A14+2*A15+3*A19+A18+2*A1+A131+A44+A50+3*A10+A11+2*A12+A56							[70]
C ₁₃ H ₁₁ N ₃ O ₄	2-cyano-6-nitro-1(2 <i>H</i>)-quinolinecarboxylic acid, ethyl ester	391.2	27.11	0	69.30	54.6	27.11	21.4
	A14+3*A15+3*A10+A12+2*A19+2*A18+A16+A50+A56+A2+A1+A169							[274]
C ₁₃ H ₁₂	diphenylmethane	298.4	19.01	0	63.7	61.9	19.0	18.5
	10*A10+A2+2*A11							[311]
C ₁₃ H ₁₂ ClN ₂ O ₂	4-chloro-2'-hydroxy-4'-methoxyazobenzene	390.0	33.7	0	86.4	69.5	33.7	27.1
	7*A10+5*A12+A1+A31+A22*D22+A32+2*A42							[152]
C ₁₃ H ₁₂ ClN ₃ S	N-2-(3-picolyl)-N'-(2-chlorophenyl) thiourea	400.2	11.2	0	28.0	72.2	11.2	28.9
	7*A10+3*A12+A41+A90+A22*D22+A11+A1							[4]
C ₁₃ H ₁₂ ClN ₃ S	N-2-(4-picolyl)-N'-(2-chlorophenyl) thiourea	441.2	44.5	0	100.9	72.2	44.5	31.9
	7*A10+3*A12+A41+A90+A22*D22+A11+A1							[4]
C ₁₃ H ₁₂ ClN ₃ S	N-2-(5-picolyl)-N'-(2-chlorophenyl) thiourea	460.2	24.2	0	52.6	72.2	24.2	33.2
	7*A10+3*A12+A41+A90+A22*D22+A11+A1							[4]
C ₁₃ H ₁₂ ClN ₃ S	N-2-(6-picolyl)-N'-(2-chlorophenyl) thiourea	449.7	27.3	0	60.7	72.2	27.3	32.5
	7*A10+3*A12+A41+A90+A22*D22+A11+A1							[4]
C ₁₃ H ₁₂ ClN ₃ S	N-2-(3-picolyl)-N'-(4-chlorophenyl) thiourea	391.2	16.8	0	42.9	72.2	16.8	28.2
	7*A10+3*A12+A41+A90+A22*D22+A11+A1							[5]
C ₁₃ H ₁₂ ClN ₃ S	N-2-(4-picolyl)-N'-(4-chlorophenyl) thiourea	460.2	35.2	0	76.5	72.2	25.2	33.2
	7*A10+3*A12+A41+A90+A22*D22+A11+A1							[5]

C ₁₃ H ₁₂ ClN ₃ S	N-2-(5-picolyl)-N'-(4-chlorophenyl) thiourea	473.7	51.1	0	107.9	72.2	51.1	34.2
	7*A10+3*A12+A41+A90+A22*D22+A11+A1							[5]
C ₁₃ H ₁₂ ClN ₃ S	N-2-(6-picolyl)-N'-(4-chlorophenyl) thiourea	464.2	40.1	0	86.4	72.2	40.1	33.5
	7*A10+3*A12+A41+A90+A22*D22+A11+A1							[5]
C ₁₃ H ₁₂ N ₂ O ₂	N-methyl-N-(4-biphenyl)nitramine	415.1	24.0	0	57.8	54.4	24.0	22.6
	9*A10+3*A12+A51+A47							[127]
C ₁₃ H ₁₂ N ₂ O ₂	2-cyano-1(2 <i>H</i>)-quinolinecarboxylic acid, ethyl ester	337.0	19.88	0	59.0	51.8	19.9	17.5
	A14+3*A15+4*A10+2*A19+2*A18+A16+A56+A2+A1+A179							[274]
C ₁₃ H ₁₂ O	2-(phenylmethyl)phenol (2-benzylphenol)	(I) 326.2	21.8	0	66.83	67.3	21.8	22.0
		(II) 288.2	17.0	0	58.99	67.3	17.0	19.4
	Independent value from another reference	(I) 325.7	23.4	0	71.85	67.3	23.4	21.9
	9*A10+A12+2*A11+A2+A31							[277, 279]
C ₁₃ H ₁₂ O	2-biphenylmethanol	324.0	19.70	0	60.80	50.8	19.70	16.5
	9*A10+2*A12+A11+A2+A30							[401]
C ₁₃ H ₁₂ O	4-biphenylmethanol	375.5	27.0	0	71.90	50.8	27.0	19.1
	9*A10+2*A12+A11+A2+A30							[401]
C ₁₃ H ₁₃ NO	1-keto-1,2,3,4-tetrahydro-6-methylcarbazole	468.5	26.9	0	57.4	54.9	26.9	25.7
	2*A14+3*A15+2*A19+2*A16+A114+A121+A11+A1+3*A10							[424]
C ₁₃ H ₁₃ N ₃ O	N-(4-methylphenyl)-N'-(2-pyridyl) urea	447.0	204.45	0	457.4	53.3 ^a	204.45	23.8
	8*A10+A11+2*A12+A41+A90							[3, 282]
	[Note: Value is too large. Most likely there is a decimal place error in the numerical value.]							
C ₁₃ H ₁₃ N ₃ S	N-2-(6-picolyl)-N'-phenylthiourea	460.7	43.5	0	94.42	70.9	43.5	32.7

		8*A10+2*A12+A41+A90+A11+A1				[6]
C ₁₃ H ₁₅ Cl ₂ N ₃	Penconazole					
332.4	33.58	0	101.02	68.9	33.58	22.9
	A1+3*A2+A3+3*A10+A11+2*A12+2*A22*D22+A14+2*A15+2*A18*B18+2*A118+A119					[175]
C ₁₃ H ₁₅ NO ₂	ethyl 4,7-dihydro-4,7-ethano-2H-isoindole-1-carboxylate					
401.8	45.4	0	113.0	69.6	45.4	28.0
	3*A14+2*A15+A121+3*A19+2*A18+A18*B18+2*A16+A38+A1+A2					[107]
C ₁₃ H ₁₇ NFe	N,N-dimethylaminomethyl ferrocene					
279.9	15.01	0	53.6	61.8	15.0	17.3
	2*A14+4*A15+9*A18*B18+A19+A2+2*A1+A43					[17]
C ₁₃ H ₁₈ Br ₂ N ₂ O	<i>trans</i> -4-[[[(2-amino-3,5-dibromophenyl)methyl]amino]cyclohexanol (Ambroxol)					
(I) 372.7	31.46	0	84.4	78.3	31.5	29.2
(II) 365.6	36.52	0	99.9	78.3	36.5	28.6
	2*A10+3*A12+A11+A2+A44+A45+2*A21+A14+3*A15+2*A16+A30*D30					[264]
C ₁₃ H ₁₈ O ₂	Ibuprofen					
347.2	25.5	0	73.4	57.5	25.5	20.0
	Independent value from another reference					
348.0	26.65	0	76.6	57.5	26.7	20.0
	3*A1+A2+4*A10+2*A11+A3+A3*B3+A36					[2,216]
C ₁₃ H ₁₈ O ₂	(S) α-methyl-4-(2-methylpropyl)benzeneacetic acid ((S)-Ibuprofen)					
324.2	18.05	0	55.7	57.5	18.1	18.6
	3*A1+A2+4*A10+2*A11+A3+A3*B3+A36					[290]
C ₁₃ H ₁₈ O ₃	3-hexyloxybenzoic acid					
343.0	22.72	0	66.2	88.6	22.7	30.4
	4*A10+2*A12+A1+5*A2+A32+A36*B36					[126]
C ₁₃ H ₁₈ O ₇	D-Salicin					
474.7	55.5	0	116.9	173.1	55.5	82.2
	A14+3*A15+A112+2*A2+5*A30*D30+A32+5*A18*B18+4*A10+A11+A12					[436]
C ₁₃ H ₂₄ O ₄	1,13-tridecanedioic acid					
386.3	49.4	0	127.9	134.7	49.4	52.0
	11*A2*B2+2*A36*B36					[298]

C ₁₃ H ₂₆ O ₂	ethyl undecanoate						
259.2	36.16	0	139.5	133.7	36.2	34.7	
	2*A1+A2+A38+9*A2*B2						[314]
C ₁₃ H ₂₈ N ₂ O	1-dodecyl urea						
275.4	1.3	4.72					
379.2	46.6	122.89	127.6	134.0	47.9	50.8	
	A1+A67+11*A2*B2						[305]
C ₁₄ H ₁₀ N ₂ O ₃	10-methyl-2-nitroacridin-9(10 <i>H</i>)-one						
561.0	37.6	0	67.02	54.2	37.6	30.4	
	7*A10+A12+A14+3*A15+4*A19+A114+A119+A1+A50						[180]
C ₁₄ H ₁₀	anthracene						
491.0	31.5	0	64.2	44.0	31.5	21.6	
	10*A10+4*A12						[180]
C ₁₄ H ₁₀ O ₂	benzil						
368.1	22.88	0	62.2	68.2	22.9	25.1	
	10*A10+2*A12+2*A35						[313]
C ₁₄ H ₁₀ O ₅	salicylsalicylic acid						
430.2	29.0	0	67.4	87.4	29.0	37.6	
	8*A10+4*A12+A36*D36+A31+A38						[236]
C ₁₄ H ₁₁ BrN ₂ S	N-(4-bromophenyl)-4 <i>H</i> -3,1-benzothiazin-2-amine						
478.3	24.5	0	51.2	67.4	24.5	32.2	
	A14+3*A15+3*A19+A118+A131+A44+8*A10+2*A12+A21						[228]
C ₁₄ H ₁₁ ClN ₂ S	N-(4-chlorophenyl)-4 <i>H</i> -3,1-benzothiazin-2-amine						
476.4	27.5	0	57.7	66.1	27.5	31.5	
	A14+3*A15+3*A19+A118+A131+A44+8*A10+2*A12+A22*D22						[228]
C ₁₄ H ₁₁ NO	N-acetylcarbazole						
349.9	15.1	0	43.2	51.7	15.1	18.1	
	8*A10+A14+2*A15+4*A19+A146+A1						[136]
C ₁₄ H ₁₁ NO	10-methylacridin-9(10 <i>H</i>)-one						
479.0	29.7	0	62.0	51.4	29.7	24.6	
	8*A10+A14+3*A15+4*A19+A114+A119+A1						[180]

C ₁₄ H ₁₁ N ₃ O ₄	2-cyano-6-nitro-1(2 <i>H</i>)-quinolinecarboxylic acid, 2-propenyl ester					
383.7	26.87	0	70.0	59.6	26.9	22.9
	A14+3*A15+3*A10+A12+2*A19+2*A18+A16+A56+A50+A2+A5+A6+A169					[274]
C ₁₄ H ₁₁ N ₃ O ₄	2-cyano-6-nitro-1(2 <i>H</i>)-quinolinecarboxylic acid, 1-propenyl ester					
389.4	26.27	0	67.5	58.1	26.3	22.6
	A14+3*A15+3*A10+A12+2*A19+2*A18+A16+A56+A50+A1+2*A6+A169					[274]
C ₁₄ H ₁₂ BrNO S	3-bromo-N-(4-methoxyphenyl)benzenecarbothioamide					
(I) 376.7	28.5	0	75.7	84.0	28.5	31.6
(II) 373.2	22.6	0	60.6	84.0	22.6	31.4
	A92+8*A10+4*A12+A1+A32+A21					[450]
C ₁₄ H ₁₂ ClNO ₂	Tolfenamic acid					
485.3	41.2	0	84.9	70.9	41.2	34.4
	7*A10+A11+4*A12+A22*D22+A36*D36+A44+A1					[418]
C ₁₄ H ₁₂ N ₂	2,9-dimethyl-1,10-phenanthroline					
435.9	17.6	0	40.4	52.2	17.6	22.8
	6*A10+4*A12+2*A11+2*A1+2*A41					[426]
C ₁₄ H ₁₂ N ₂ O ₄	N-methylthalidomide					
432.2	18.12	0	41.9	66.0	18.1	28.5
	4*A10+2*A14+5*A15+2*A19+2*A128+A16+A1					[73]
C ₁₄ H ₁₂ O	9-fluorenemethanol					
376.6	26.27	0	69.8	44.9	26.3	16.9
	8*A10+A14+2*A15+4*A19+A2+A16+A30					[161]
C ₁₄ H ₁₂ O ₃	2-hydroxy-4-methoxybenzophenone					
336.7	21.77	0	64.7	76.4	21.8	25.7
	8*A10+4*A12+A1+A31+A35+A32					[379]
C ₁₄ H ₁₂ O ₅	4,9-dimethoxy-7-methyl-5 <i>H</i> -furo[3,2 <i>g</i>][1]benzopyran-5-one (Khellin)					
(I) 423.5	27.90	0	65.9	79.3	27.9	33.6
(II) 426.5	32.32	0	75.8	79.3	32.3	33.8
	2*A14+5*A15+3*A1+5*A19+2*A32+A18+2*A18*B18+2*A112+A114					[56]
C ₁₄ H ₁₃ NO	N,N-diphenylacetamide					
374.4	23.4	0	62.5	65.4	23.4	24.5

	10*A10+2*A12+A1+A59					[136]
C ₁₄ H ₁₃ N ₃ O ₄	2-cyano-6-nitro-1(2 <i>H</i>)-quinolinecarboxylic acid, propyl ester					
372.2	24.99	0	67.2	61.7	25.0	23.0
	A14+3*A15+3*A10+A12+2*A19+2*A18+A16+2*A2+A1+A56+A50+A179					[274]
C ₁₄ H ₁₃ N ₃ O ₄	2-cyano-6-nitro-1(2 <i>H</i>)-quinolinecarboxylic acid, 1-methylethyl ester					
402.0	27.75	0	69.0	55.3	27.8	22.2
	A14+3*A15+3*A10+A12+2*A19+2*A18+A16+2*A1+A3*B3+A56+A50+A179					[274]
C ₁₄ H ₁₄ ClN ₂ O ₂	4-chloro-2'-hydroxy-4'-ethoxyazobenzene					
421.0	34.3	0	81.47	76.6	34.3	32.3
	7*A10+5*A12+A1+A31+A2+A22*D22+A32+2*A42					[152]
C ₁₄ H ₁₄ ClN ₃ S	N-2-(4,6-lutidyl)-N'-(2-chlorophenyl) thiourea					
467.2	42.2	0	90.3	72.8	42.2	34.0
	6*A10+3*A12+2*A11+A41+2*A1+A90+A22*D22					[4]
C ₁₄ H ₁₄ ClN ₃ S	N-2-(4,6-lutidyl)-N'-(4-chlorophenyl) thiourea					
499.7	66.5	0	133.1	72.8 ^a	66.5	36.4
	6*A10+3*A12+2*A11+A41+2*A1+A90+A22*D22					[5]
C ₁₄ H ₁₄ F ₃ NO ₂	4-trifluoromethyl-7-(<i>N,N</i> -diethylamino)coumarin					
360.0	23.3	0	64.7	66.5	23.3	23.9
	A14+3*A15+A115+A18*B18+3*A19+3*A10+A12+A43+2*A1+2*A2+A4*B4+3*A25					[118]
C ₁₄ H ₁₄ N ₂ O ₂	N-methyl-N-nitro-4-(phenylmethyl)benzenamine					
329.6	21.7	0	65.8	72.6	21.7	23.9
	8*A10+3*A12+A11+2*A1+A47+A51					[127]
C ₁₄ H ₁₄ N ₂ O ₃	2-cyano-6-methoxy-1(2 <i>H</i>)-quinolinecarboxylic acid, ethyl ester					
359.1	22.37	0	62.3	59.2	22.4	21.3
	A14+3*A15+3*A10+A12+2*A19+2*A18+A16+2*A1+A2+A56+A32+A169					[274]
C ₁₄ H ₁₄ O ₅	8-(hydroxymethyl)-6-methyl-2-oxo-2 <i>H</i> -1-benzopyran-3-carboxylic acid, ethyl ester					
415.6	2.96	7.12				
429.8	29.58	68.82	75.9	71.2	32.5	30.6
	A14+3*A15+3*A19+A18+A115+2*A10+2*A11+2*A1+A2+A30*C30+A38					[129]
C ₁₄ H ₁₄ O ₆	8-(hydroxymethyl)-6-methoxy-2-oxo-2 <i>H</i> -1-benzopyran-3-carboxylic acid,					

	ethyl ester						
431.9	36.42	0	84.3	76.0	36.4	32.8	
	A14+3*A15+3*A19+A18+A115+2*A10+2*A11+A1+A30*C30+A36*C36+A2 [129]						
C ₁₄ H ₁₄ S ₂	benzyl disulfide						
341.7	44.70	0	130.8	85.1	44.70	29.1	
	10*A10+2*A11+A85+2*A2 [428]						
C ₁₄ H ₁₅ N ₃ S	N-2-(4,6-lutidyl)-N'-phenylthiourea						
489.7	50.9	0	103.9	64.0	50.9	31.3	
	7*A10+3*A12+2*A11+A41+2*A1+A90 [6]						
C ₁₄ H ₁₅ N ₃ S	N-2-(6-picolyl)-N'-2-tolylthiourea						
468.7	44.1	0	94.1	64.0	44.1	30.0	
	7*A10+3*A12+2*A11+A41+2*A1+A90 [91]						
C ₁₄ H ₁₅ N ₃ S	N-2-(6-picolyl)-N'-3-tolylthiourea						
460.7	33.2	0	72.1	64.0	33.2	29.5	
	7*A10+3*A12+2*A11+A41+2*A1+A90 [91]						
C ₁₄ H ₁₅ N ₃ S	N-2-(6-picolyl)-N'-4-tolylthiourea						
492.2	47.2	0	95.9	64.0	47.2	31.5	
	7*A10+3*A12+2*A11+A41+2*A1+A90 [91]						
C ₁₄ H ₁₆ ClN ₃ O	Metazachlor						
(I) 356.2	19.7	0	55.3	64.2	19.7	22.9	
(II) 353.2	23.0	0	65.1	64.2	23.0	22.7	
(III) 349.2	26.6	0	76.2	64.2	26.6	22.4	
	A14+2*A15+2*A18*B18+A18+A119+A118+2*A2+A59+A22*D22+2*A1+2*A11+A12+3*A10 [259]						
C ₁₄ H ₁₇ N ₅ O ₃	Pipemidic acid						
529.9	32.85	0	62.0	59.9	32.9	31.7	
	2*A14+6*A15+3*A19+A18*B18+A114+2*A119+A121+2*A118+A10+A12+A1+A36*D36 [260]						
C ₁₄ H ₁₈ Fe	n-butylferrocene						
281.5	21.43	0	76.1	80.6	21.4	22.7	
	2*A14+4*A15+9*A18*B18+A19+A1+3*A2 [16]						

C ₁₄ H ₁₈ N ₂ O ₅	3,5-dinitro-2,6-dimethyl-4- <i>tert</i> -butylacetophenone (musk ketone)						
408.5	23.81	0	58.3	59.5	23.8	24.3	
	3*A11+3*A12+6*A1+A35+2*A50+A4						[234]
C ₁₄ H ₁₉ N ₂ O ₂	(1RS, 2RS)-1-(4-chlorophenoxy)-3,3-dimethyl-1-(1 <i>H</i> -1,2,4-triazol-1-yl)-butan-2-ol (Triadimenol)						
(I) 411.2	32.0	0	77.8	85.7	32.0	35.2	
(II) 406.2	33.1	0	81.5	85.7	33.1	34.8	
(III) 385.2	25.1	0	65.2	85.7	25.1	33.0	
	A14+2*A15+2*A118+A119+A2+2*A3*B3+A30*D30+A4+3*A1+A32+2*A12+4*A10+A22*D22						[65]
C ₁₄ H ₁₉ N ₂ O ₂	(1RS,2SR)-1-(4-chlorophenoxy)-3,3-dimethyl-1-(1 <i>H</i> -1,2,4-triazol-1-yl)-butan-2-ol (Triadimenol)						
406.2	33.2	0	81.7	85.7	33.2	34.8	
	A14+2*A15+2*A118+A119+A2+2*A3*B3+A30*D30+A4+3*A1+A32+2*A12+4*A10+A22*D22						[65]
C ₁₄ H ₂₀ N ₂ O ₂	1-(1 <i>H</i> -indol-4-yloxy)-3-isopropylamino-2-propanol (Pindolol)						
443.8	58.0	0	130.7	79.8	58.0	35.4	
	Independent value from another reference						
423.6	60.6	0	143.1	79.8	60.6	33.8	
	3*A10+A12+A14+2*A15+A18+A18*B18+2*A19+A121+2*A1+2*A2+2*A3*B3+A30*D30+A32+A44						[257, 419]
C ₁₄ H ₂₀ O ₂	3,5-di- <i>tert</i> -butyl- <i>o</i> -quinone						
387.9	26.53	0	68.4	48.4	26.5	18.8	
	6*A1+A14+3*A15+A18+A18*B18+2*A19+2*A4+2*A114						[313]
C ₁₄ H ₂₂ N ₂ O ₃	Atenolol						
426.1	38.7	0	90.8	98.9	38.7	42.1	
	2*A1+3*A2+2*A3*B3+4*A10+A11+A12+A44+A30*D30+A32+A61						[419]
C ₁₄ H ₂₂ N ₄ O ₆	N,N'- <i>bis</i> (2-oxo-3-oxazolidin-3-ylcarbonyl)-1,6-hexanediamine (N,N'-1,6-hexanediylylbis[2-oxo-3-oxazolidinecarboxamide])						
400.8	8.9	0	22.21	116.8 ^a	8.9	46.8	
	2*A14+4*A15+2*A126+2*A60+6*A2						[143]
C ₁₄ H ₂₄ N ₂	tetradecanedinitrile						
261.1	1.77	6.78					

	309.6	40.17	129.75	136.5	147.0	41.94	45.5
		12*A2*B2+2*A56					[402]
C ₁₄ H ₂₆ O ₄		1,14-tetradecanedioic acid					
	397.3	56.5	0	142.2	144.0	56.5	57.2
		12*A2*B2+2*A36*B36					[298]
C ₁₄ H ₂₈ N ₂ O ₂		N,N,N',N'-tetrapropylloxamide					
	317.2	21.0	0	66.2	104.8	21.0	33.2
		4*A1+8*A2+ 2*A59					[27]
C ₁₄ H ₂₈ N ₂ O ₂		tetradecandiamide					
	469.3	77.45	0	165.0	167.4	77.5	78.6
		12*A2*B2+2*A61					[357]
C ₁₄ H ₂₈ O ₆		2-ethylhexyl α-D-glucoside					
	341.2	33.47	98.09				
	387.2	3.56	9.19	107.3	127.4	37.0	49.3
		A14+3*A15+5*A16*B16+A112+4*A30*D30+6*A2+2*A1+A32+A3					[122]
C ₁₄ H ₂₈ O ₆		2-ethylhexyl β-D-glucoside					
	330.2	10.88	0	33.0	127.4 ^a	10.9	42.1
		A14+3*A15+5*A16*B16+A112+4*A30*D30+6*A2+2*A1+A32+A3					[122]
C ₁₄ H ₃₀ N ₂ O		1-tridecyl urea					
	261.6	1.5	5.73				
	306.5	2.8	9.14				
	384.6	46.0	119.60	134.47	143.3	50.3	55.1
		A1+A67+12*A2*B2					[305]
C ₁₅ H ₁₀ O ₄		5,7-dihydroxy-2-phenyl-4H-1-benzopyran-4-one (Chrysin)					
	558.2	39.2	0	70.2	91.2	39.2	50.9
		A14+3*A15+A112+A114+4*A19+7*A10+3*A12+3*A30*D30					[384]
C ₁₅ H ₁₀ O ₇		2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-1-benzopyran-4-one (Quercetin)					
	595.2	41.5	0	69.72	106.0	41.5	63.1
		A14+3*A15+A112+A114+4*A19+5*A10+5*A12+5*A30*D30					[384]
C ₁₅ H ₁₁ Cl ₂ N ₂ O ₂		Lorazepam					
	446.5	92.57	0	207.3	82.5 ^a	92.6	36.8

		A14+4*A15+A124+3*A19+A16+A118+A30*D30+2*A22*D22+3*A12+7*A10					[25]
C ₁₅ H ₁₂ ClN ₂ O ₂	Oxazepam						
467.5	84.11	0	179.9	82.5 ^a	84.1	38.6	
	A14+4*A15+A124+3*A19+A16+A118+A30*D30+A22*D22+2*A12+8*A10					[25]	
C ₁₅ H ₁₂ NO	Carbamazepine						
(I) 466.7	25.52	0	54.7	55.3	25.5	25.8	
(II) 464.4	26.82	0	57.8	55.3	26.8	25.7	
(III) 464.7	24.89	0	53.6	55.3	24.9	25.7	
	A14+4*A15+2*A18+4*A19+A170+8*A10					[154]	
C ₁₅ H ₁₂ N ₂ O ₂	5,5-diphenyl-2,4-imidazolidinedione (Phenytoin)						
570.8	47.08	0	82.5	96.3	47.1	55.0	
	A14+2*A15+2*A124+A20+2*A11+10*A10					[113]	
C ₁₅ H ₁₂ O ₅	2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one (Naringenin)						
523.2	39.8	0	76.1	84.1	39.8	44.0	
	A14+3*A15+2*A19+A16+A112+A114+3*A12+A11+6*A10+3*A30*D30					[384]	
C ₁₅ H ₁₃ ClN ₂ S	N-(2-methyl-4-chlorophenyl)-4H-3,1-benzothiazin-2-amine						
495.8	17.5	0	35.3	71.1	17.5	35.3	
	A14+3*A15+3*A19+A131+A118+8*A10+A11+A12+A2+A44+A22*D22					[228]	
C ₁₅ H ₁₃ FO ₂	2-fluoro- α -methyl[1,1'-biphenyl]-4-acetic acid (Flurbiprofen)						
386.7	27.9	0	72.2	67.7	27.9	26.2	
	8*A10+3*A12+A11+A1+A36*B36+A24+A3*B3					[275]	
C ₁₅ H ₁₃ NO	2,10-dimethylacridin-9(10H)-one						
426.0	22.4	0	52.6	52.0	22.4	22.2	
	7*A10+A11+A14+3*A15+4*A19+A114+A119+2*A1					[180]	
C ₁₅ H ₁₃ NO	10-ethylacridin-9(10H)-one						
434.0	27.5	0	63.4	58.5	27.5	25.4	
	A14+3*A15+4*A19+A114+A119+8*A10+A1+A2					[180]	
C ₁₅ H ₁₃ NO ₃	5-benzoyl-2,3-dihydro-1H-pyrrolizine-1-carboxylic acid (Ketorolac)						
(I) 431.2	28.62	0	66.4	84.1	28.62	36.2	
(II) 430.2	171.74	0	399.2	84.1 ^a	171.74	36.2	
	Value for (II) seems much too large in comparison with fusion enthalpies of the other two						

	371.0	29.8	0	80.3	83.7	29.8	31.1
				7*A10+5*A12+A1+A31+2*A2+A22*D22+A32+2*A42			[152]
C ₁₅ H ₁₆ N ₂ O ₂		2-cyano-1(2 <i>H</i>)-quinolinecarboxylic acid, butyl ester					
	347.5	22.50	0	64.8	66.0	22.5	22.9
		A14+3*A15+4*A10+2*A19+2*A18+A16+3*A2+A1+A56+A169					[274]
C ₁₅ H ₁₆ N ₂ O ₂ S		N,N'-bis(3-methoxyphenyl)thiourea					
	405.2	43.83	0	108.17	81.6	43.83	33.1
		8*A10+4*A12+2*A1+2*A32+A90					[262]
C ₁₅ H ₁₆ N ₂ O ₃		N,N'-bis(3-methoxyphenyl)urea					
	443.2	36.76	0	83.01	65.7	36.76	29.1
		8*A10+4*A12+2*A1+2*A32+A66					[262]
C ₁₅ H ₁₆ N ₂ O ₃		2-cyano-6-methoxy-1(2 <i>H</i>)-quinolinecarboxylic acid, propyl ester					
	339.9	15.60	0	45.9	66.3	15.6	22.5
		A14+3*A15+3*A10+A12+2*A19+2*A18+A16+2*A2+2*A1+A56+A32+A169					[274]
C ₁₅ H ₁₆ N ₄ O ₆		2,4-bis(2-oxo-3-oxazolidin-3-ylcarbonylamino)toluene					
	479.5	5.2	0	10.84		5.2	
		prediction not made					[143]
C ₁₅ H ₁₇ ClN ₄		α -butyl- α -(4-chlorophenyl)-1 <i>H</i> -1,2,4-triazole-1-propanenitrile (Myclobutanil)					
	348.8	30.93	0	88.7	91.4	30.9	31.9
		A14+2*A15+A118+A119+A1+4*A2+A4*B4+A56+4*A10+A11+A12+A22*D22					[286]
C ₁₅ H ₁₈ FeOS ₂		1,4,6-oxadithiacyclooctan-5-ylferrocene					
	383.3	24.4	0	63.7	80.9	24.4	31.0
		A14+5*A15+A112+2*A131+A16+2*A14+4*A15+A19+9*A18*B18+A179					[130]
C ₁₅ H ₂₀ N ₄ O ₄		1,1'-(1,5-pentanediy)-bis-thymine					
	524.0	32.03	0	61.1	91.0	32.0	47.7
		5*A2+2*A125+2*A124+2*A14+6*A15+2*A1+2*A19+2*A18*B18					[110]
C ₁₅ H ₂₂ O ₃		3-octyloxybenzoic acid					
	347.1	33.12	0	95.42	102.8	33.12	35.7
		4*A10+2*A12+A1+A32+A36*B36+7*A2					[126]
C ₁₅ H ₂₂ O ₃		3,5-di- <i>tert</i> -butylsalicylic acid					
	437.5	22.92	0	52.4	53.1	22.92	23.2

		$6*A1+2*A10+2*A11+2*A12+2*A4+A31+A36*B36$					[134]
$C_{15}H_{22}O_5$	octahydro-3,6,9-trimethyl-3,12-epoxy-12 <i>H</i> -pyrano[4,3- <i>j</i>]-1,2-benzodioxepin-10(3 <i>H</i>)-one						
(I)	428.2	22.80	0	53.3		22.8	
(II)	428.1	23.41	0	54.7		23.4	
	prediction not made					[92]	
$C_{15}H_{23}N_3O_2$	N-caprylpyrazinamide						
	360.4	50.58	0	140.3	138.9	50.58	
	$3*A10+A12+2*A41+A71+8*A2*B2+A1$					[86]	
$C_{15}H_{24}N_2O_3$	4-(butylamino)-2-hydroxybenzoic acid, 2-(dimethylamino)ethyl ester (Salicaine)						
	319.4	26.8	0	83.9	88.5	26.8	
	$3*A1+5*A2+3*A10+3*A12+A38+A31+A43+A44$					[353]	
$C_{15}H_{30}O_2$	ethyl tridecanoate						
	272.4	40.7	0	149.4	152.3	40.7	
	$2*A1+A2+A38+11*A2*B2$					[314]	
$C_{15}H_{32}N_2O$	1-tetradecyl urea						
	227.1	1.0	4.40				
	369.2	1.7	4.60				
	387.4	50.9	131.39	140.4	152.6	53.6	
	$A1+A67+13*A2*B2$					[305]	
$C_{15}H_{32}O$	1-pentadecanol						
	316.4	29.6	0	93.6	149.5	29.6	
	$A1+14*A2*B2+A30$					[208]	
$C_{16}H_{10}ClN_3O$	1-[(2-chloro-3-pyridinyl)carbonyl]-1,2-dihydro-2-quinolinecarbonitrile						
	489.8	50.89	0	103.9	66.9	50.9	
	$A14+3*A15+2*A19+2*A18+A16+7*A10+2*A12+A41+A146+A56+A22*D22$					[274]	
$C_{16}H_{11}N_3O$	1-[(3-pyridinyl)carbonyl]-1,2-dihydro-2-quinolinecarbonitrile						
	412.5	31.01	0	75.2	65.6	31.0	
	$A14+3*A15+2*A19+2*A18+A16+8*A10+A12+A41+A146+A56$					[274]	
$C_{16}H_{12}$	[2.2]-paracyclophane-1,9-diene						
	505.9	30.71	0	60.7	34.3	30.7	
	$A14+9*A15+4*A19+8*A18+4*A10$					[196]	

C ₁₆ H ₁₂	2-phenylnaphthalene						
373.5	17.90	0	47.93	58.8	17.90	22.0	
	12*A10+4*A12					[406]	
C ₁₆ H ₁₂ O ₂	5-hydroxymethylene-5 <i>H</i> -6,7-dihydrodibenzo[a,c]cyclohepten-6-one						
357.7	16.9	0	47.3	66.1	16.9	23.7	
	A14+4*A15+5*A19+A114+8*A10+A6*B6+A30*B30					[370]	
C ₁₆ H ₁₂ S ₂	2,6-diphenyl-1,4-dithiin						
(I) 336.6	20.9	0	62.1	78.6	20.9	26.4	
(II) 350.7	24.6	0	70.2	78.6	24.6	27.6	
	10*A10+2*A12+A14+3*A15+2*A18*B18+2*A19+2*A131					[258]	
C ₁₆ H ₁₃ ClN ₂ O	Diazepam						
403.6	25.49	0	63.2	68.1	25.49	27.5	
	A14+4*A15+8*A10+2*A12+A1+A118+A125+3*A19+A22*D22					[25]	
C ₁₆ H ₁₃ NO ₃	1-[(4-nitrophenyl)ethynyl]-4-ethoxybenzene						
388.1	26.02	0	67.0	67.7	26.02	26.3	
	8*A10+4*A12+A50+A2+A1+2*A9+A32					[153]	
C ₁₆ H ₁₃ NO ₇	2-acetoxybenzoic acid, 3'-(nitrooxymethyl)phenyl ester						
(I) 335.2	33.79	0	100.8	91.6	33.8	30.7	
(II) 328.5	26.83	0	81.7	91.6	26.8	30.1	
	8*A10+3*A12+A11+2*A38+A2+A1+A55					[173]	
C ₁₆ H ₁₄	[2.2]-paracyclophane-1-ene						
469.9	17.61	0	37.5	37.5	17.6	17.6	
	A14+9*A15+4*A19+6*A18+4*A10					[196]	
C ₁₆ H ₁₄ N ₂	1-methyl-3,5-diphenylpyrazole						
332.9	17.46	0	52.5	54.2	17.5	18.0	
	A14+2*A15+2*A19+2*A119+A1+10*A10+2*A12					[61]	
C ₁₆ H ₁₄ N ₂ OS	N-(4-acetylphenyl)-4 <i>H</i> -3,1-benzothiazin-2-amine						
436.2	16.1	0	36.9	36.9	16.1	16.1	
	+A14+3*A15+A182+2*A19+8*A10+2*A12+A1+A35					[228]	
C ₁₆ H ₁₄ N ₂ O ₃ S	4-(5-methyl-3-phenyl-4-isoxazolyl)benzenesulfonamide (Valdecocixib)						
446.4	30.35	0	68.0	92.5	30.4	41.3	

		A14+2*A15+3*A19+A118+A112+9*A10+3*A12+A1+A96				[241]
C ₁₆ H ₁₄ O	2,3:6,7-dibenzocycloocta-2,6-dien-1-one					
366.6	17.2	0	46.9	66.5	17.2	24.4
	A14+5*A15+4*A19+A35+8*A10					[32]
C ₁₆ H ₁₄ O	2,3:7,8-dibenzocycloocta-2,7-dien-1-one					
420.0	27.8	0	66.2	66.5	27.8	27.9
	A14+5*A15+4*A19+A35+8*A10					[32]
C ₁₆ H ₁₄ O ₃	Fenbufen					
462.9	41.1	0	88.8	79.1	41.1	36.6
	9*A10+3*A12+2*A2+A35+A36*B36					[430]
C ₁₆ H ₁₄ O ₆	2,3-dihydro-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4H-1-benzopyran-4-one (Hesperitin)					
499.2	35.9	0	71.9	87.7	35.9	43.8
	A14+3*A15+A114+A112+2*A19+A16+5*A10+5*A12+A1+A32+3*A31					[384]
C ₁₆ H ₁₅ BrO	4-bromo-4'-(3-butenyloxy)-1,1'-biphenyl					
324.2	13.3	41.02				
396.8	15.8	39.82	80.8	88.2	29.1	35.0
	8*A10+4*A12+A32+2*A2+A21+A5+A6					[227]
C ₁₆ H ₁₅ NO ₄	2-(4-nitrophenyl)-1-(4-ethoxyphenyl)ethanone					
390.3	28.20	0	72.3	85.9	28.2	33.5
	A1+2*A2+8*A10+3*A12+A11+A32+A35+A50					[153]
C ₁₆ H ₁₆ N ₂ O ₂	N,N'-bis(salicylaldehydo)ethylenediimine					
397.9	34.09	0	85.7	88.4	34.1	35.2
	8*A10+4*A12+2*A2+2*A6*B6+2*A42+2*A31					[253]
C ₁₆ H ₁₆ N ₂ O ₄	N-propylthalidomide					
409.2	27.28	0	66.7	80.2	27.28	32.8
	4*A10+2*A14+5*A15+2*A19+2*A128+A16+A1+2*A2					[73]
C ₁₆ H ₁₆ O	6-hydroxymethyl-5,6-dihydro-7H-dibenzo[a,c]cycloheptane					
405.7	25.9	0	63.8	52.3	25.9	21.2
	A14+4*A15+8*A10+4*A19+A16+A30+A2					[333]
C ₁₆ H ₁₆ O	5-hydroxymethyl-5,6-dihydro-7H-dibenzo[a,c]cycloheptane					

	352.5	16.0	0	45.4	52.3	16.0	18.4
	A14+4*A15+8*A10+4*A19+A16+A30+A2						[333]
C ₁₆ H ₁₆ O ₂	<i>trans</i> -9,10-bishydroxymethyl-9,10-dihydrophenanthrene						
	450.8	30.3	0	67.2	74.6	30.3	33.6
	A14+3*A15+8*A10+4*A19+2*A16+2*A2+2*A30*B30						[333]
C ₁₆ H ₁₆ O ₂	<i>trans</i> -5-hydroxymethyl-5,6-dihydro-7 <i>H</i> -dibenzo[a,c]cycloheptan-6-ol						
	460.2	31.8	0	69.1	71.2	31.8	32.8
	A14+4*A15+8*A10+4*A19+A2+2*A16+2*A30*B30						[333]
C ₁₆ H ₁₇ N ₃ O ₃	6-(acetylamino)-2-cyano-1(2 <i>H</i>)-quinolinecarboxylic acid, 1-methylethyl ester						
	377.4	12.66	0	33.6	50.1	12.7	18.9
	A14+3*A15+3*A10+A12+2*A19+2*A18+A16+A60+A56+3*A1+A3+A169						[274]
C ₁₆ H ₁₈ N ₂ OS	N-[(3-methoxyphenyl)methyl]-N'-(phenylmethyl)thiourea						
	345.0	21.02	0	60.9	84.2	21.0	29.1
	9*A10+A12+2*A11+2*A2+A1+A32+A90						[262]
C ₁₆ H ₁₈ N ₂ O ₃	2-cyano-6-methoxy-1(2 <i>H</i>)-quinolinecarboxylic acid, 2-methylpropyl ester						
	346.4	24.45	0	70.6	60.4	24.5	20.9
	A14+3*A15+3*A10+A12+2*A19+2*A18+A16+3*A1+A2+A3+A56+A32+A169						[274]
C ₁₆ H ₂₀ N ₄ O ₃ S	N-[(1-methylethyl)amino]carbonyl]-4-[(3'-methylphenyl)amino]-3-pyridinesulfonamide (Torasemide)						
							[56211-40-6]
(I)	434.7	37.2	0	85.6	81.7	37.2	35.5
(II)	430.0	29.0	0	67.4	81.7	29.0	35.1
	7*A10+A11+3*A12+A41+3*A1+A3*B3+A41+A60+A95						[83]
C ₁₆ H ₂₁ N	4-(<i>trans</i> -4-propylcyclohexyl)benzotrile						
	316.3	20.4	64.4				
	319.0	1.1	3.5	67.9	77.1	21.5	24.6
	4*A10+A12+A11+A14+3*A15+2*A2+A1+2*A16+A56						[43]
C ₁₆ H ₂₂ N ₄ O ₄	5-[[3,5-dimethoxy-4-(2-methoxyethoxy)phenyl]methyl]-2,4-pyrimidinediamine (Tetroxoprin)						
	423.3	46.36	0	109.5	123.0	46.4	52.1
	3*A10+5*A12+2*A11+2*A41+2*A45+3*A2+3*A1+4*A32						[87]
C ₁₆ H ₂₄ N ₂ OS	2-[(diethylamino)thioxomethyl]-N,N-diethylbenzamide						
	353.5	28.79	0	81.4	88.7	28.8	31.4

		4*A1+4*A2+A59+A175+2*A12+4*A10					[345]	
C ₁₆ H ₂₄ N ₂ S ₂	N,N,N',N'-tetraethyl-1,2-benzenedicarbothiamide	388.4	23.39	0	60.2	86.4	23.4	33.6
		4*A10+2*A12+4*A1+4*A2+2*A175					[345]	
C ₁₆ H ₃₀ O ₄	1,16-hexadecanedioic acid	395.4	52.2	0	132.0	162.6	52.2	64.3
		14*A2*B2+2*A36*B36					[298]	
C ₁₆ H ₃₃ NO	hexadecanamide	355.5	10.4	29.25				
		376.0	45.4	120.74	150.0	175.7	55.8	66.1
		A1+14*A2*B2+A61					[391]	
C ₁₆ H ₃₄ O	1-hexadecanol	321.6	33.1	0	103.0	158.8	33.1	51.1
	Independent value from another reference	322.2	57.7	0	179.2	158.8	57.7	51.2
		A1+15*A2*B2+A30					[208, 432]	
C ₁₆ H ₃₆ O ₃ Si ₂	11-(1,1,3,3-tetramethyldisiloxanyl)undecanoic acid, methyl ester	233.3	23.5	0	100.7		23.5	
	prediction not made						[343]	
C ₁₇ H ₁₀ ClN ₃ O ₃	1-(4-chlorobenzoyl)-1,2-dihydro-6-nitro-2-quinolinecarbonitrile	430.5	25.62	0	59.5	66.2	25.6	28.5
		A14+3*A15+2*A19+2*A18+A16+A146+7*A10+3*A12+A56+A50+A22*D22					[274]	
C ₁₇ H ₁₁ ClN ₂ O ₂	2-cyano-1(2 <i>H</i>)-quinolinecarboxylic acid, 4-chlorophenyl ester	424.2	37.19	0	87.7	96.8	37.2	41.1
		A14+3*A15+8*A10+2*A12+2*A19+2*A18+A16+3*A2+A1+A56+A22*D22+A169					[274]	
C ₁₇ H ₁₂ N ₂ O ₂	2-cyano-1(2 <i>H</i>)-quinolinecarboxylic acid, phenyl ester	399.0	31.52	0	79.0	95.5	31.5	38.1
		A14+3*A15+9*A10+A12+2*A19+2*A18+A16+3*A2+A1+A56+A169					[274]	
C ₁₇ H ₁₄ F ₃ N ₃ O ₂ S	4-[5-(3-methylphenyl)-3-(trifluoromethyl)-1 <i>H</i> -pyrazol-1-yl]benzenesulphonamide (Celecoxib)							

	436.0	34.35	0	78.8	84.7	34.4	36.9
	A14+2*A15+2*A19+A18+A118+A119+8*A10+A11+3*A12+A96+A1+3*A26*D26+A4*B4						[156]
C ₁₇ H ₁₄ FeO		benzoylferrocene					
	380.7	29.9	0	78.5	70.8	29.9	26.9
	2*A14+4*A15+9*A18*B18+A19+5*A10+A12+A179+A35						[378]
C ₁₇ H ₁₄ O		2:3,6:7-dibenzobicyclo[3.2.2]nona-2,6-dien-4-one					
	383.2	10.9	0	28.4	57.1	10.9	21.9
	2*A14+3*A15+4*A19+2*A16+A114+8*A10						[370]
C ₁₇ H ₁₄ O ₄ S		Rofecoxib					
	482.1	11.98	0	24.9	80.4	12.0	38.8
	9*A10+3*A12+A1+A88+A14+2*A15+2*A19+A115						[326]
C ₁₇ H ₁₅ NO ₂		1-[(4-nitrophenyl)ethynyl]-4-propylbenzene					
	351.3	23.26	0	66.2	70.1	23.3	24.6
	8*A10+4*A12+A50+2*A2+A1+2*A9						[153]
C ₁₇ H ₁₅ NO ₃		1-[(4-nitrophenyl)ethynyl]-4-propoxybenzene					
	377.0	31.42	0	83.3	74.8	31.4	28.2
	8*A10+4*A12+A50+2*A2+A1+2*A9+A32						[153]
C ₁₇ H ₁₆ Fe		(phenylmethyl)ferrocene					
	349.9	26.8	0	76.6	71.2	26.8	24.9
	2*A14+4*A15+9*A18*B18+A19+A2+5*A10+A11+A179						[378]
C ₁₇ H ₁₆ N ₂ O ₄		5-phenoxymethyl-3-phenylcarbamoyl-2-oxazolidone					
	415.9	12.9	0	31.0	107.9 ^a	12.9	44.9
	10*A10+2*A12+A14+2*A15+A126+A60+A32+A2						[143]
C ₁₇ H ₁₇ NO ₄		2-(4-nitrophenyl)-1-(4-propoxyphenyl)ethanone					
	372.4	31.97	0	85.9	93.0	32.0	34.6
	A1+3*A2+8*A10+3*A12+A11+A32+A35+A50						[153]
C ₁₇ H ₁₈ ClNO ₂ S		N-[4-chloro-3-[(3-methyl-2-butenyl)oxy]phenyl]-2-methyl-3-furancarbothiamide					
	400.8	36.94	0	92.2	92.2	36.9	37.0
	A14+2*A15+2*A19+A18+A18*B18+A112+3*A1+A2+A32+A7+A6+A174+A22*D22						[105]

C ₁₇ H ₁₈ N ₂ O ₃ S	4-methoxy-N-[[[(3-methoxyphenyl)methyl]amino]thioxomethyl]benzamide	389.2	31.02	0	79.7	79.7	31.0	31.0
								[262]
	8*A10+A11+3*A12+2*A1+A2+A32+A60+A174							
C ₁₇ H ₁₉ NO ₄	Fenoxycarb	326.3	26.98	0	82.68	100.2	26.98	32.7
								[316]
	9*A10+3*A12+2*A32+3*A2+A1+A69							
C ₁₇ H ₁₉ N ₃ O ₃	6-(acetylamino)-2-cyano-1(2H)-quinolinecarboxylic acid, 2-methylpropyl ester	404.6	19.83	0	49.0	57.2	19.8	23.1
								[274]
	A14+3*A15+3*A10+A12+2*A19+2*A18+A16+A60+A56+A2+3*A1+A3+A169							
C ₁₇ H ₁₉ N ₃ O ₃	6-(acetylamino)-2-cyano-1(2H)-quinolinecarboxylic acid, butyl ester	436.1	36.44	0	83.6	70.2	36.4	30.6
								[274]
	A14+3*A15+3*A10+A12+2*A19+2*A18+A16+A60+A56+3*A2+2*A1+A169							
C ₁₇ H ₂₀ N ₂ O ₂ S	N,N'-bis[(3-methoxyphenyl)methyl]thiourea	354.7	33.22	0	93.7	91.6	33.2	32.5
								[262]
	8*A10+2*A12+2*A11+2*A2+2*A1+2*A32+A90							
C ₁₇ H ₂₂ FeO ₂ S ₂	1,9-dioxa-4,6-dithiacycloundecan-5-ylferrocene	371.7	29.4	0	79.1	93.2	29.4	34.6
								[130]
	3*A14+12*A15+9*A18*B18+A19+A179+2*A112+2*A131+A16							
C ₁₇ H ₂₆ O ₃	3-decyloxybenzoic acid	345.1	33.88	0	98.2	136.8	33.9	47.2
								[126]
	4*A10+2*A12+A32+A1+9*A2*B2+A36*B36							
C ₁₇ H ₂₈ N ₂ OS	N-[(3-methoxyphenyl)methyl]-N'-octylthiourea	350.7	37.94	0	108.2	117.0	37.9	41.0
								[262]
	4*A10+A11+A12+A32+2*A1+8*A2+A90							
C ₁₇ H ₃₄ O ₂	methyl hexadecanoate	302.2	58.1	0	192.3	173.1	58.1	52.3
	Independent value from another reference							
		305.2	56.0	0	183.5	173.1	56.0	52.8
								[193, 245]
	2*A1+14*A2*B2+A38							
C ₁₇ H ₃₆ O	1-heptadecanol							

	326.6	37.0	0	113.3	168.1	37.0	54.9
	Independent values from another reference						
	323.6	25.2	0	78.0	168.1	25.2	54.4
	326.6	37.0	0	113.3	168.1	37.0	54.9
	A1+16*A2*B2+A30						[208, 299]
C ₁₇ H ₃₆ O	4-heptadecanol						
	311.5	35.7	0	114.6	152.9	35.7	47.6
	Note: Authors report the sum of the fusion enthalpy plus all phase transitions above 298 K						
	2*A1+2*A2+A30+12*A2*B2+A3*B3						[346]
C ₁₇ H ₃₆ O	6-heptadecanol						
	315.8	49.0	0	155.2	157.3	49.0	49.7
	Note: Authors report the sum of the fusion enthalpy plus all phase transitions above 298 K						
	2*A1+A30+A3*B3+14*A2*B2						[346]
C ₁₇ H ₃₆ O	7-heptadecanol						
	314.4	28.8	0	91.6	157.3 ^a	28.8	49.4
	Note: Authors report the sum of the fusion enthalpy plus all phase transitions above 298 K						
	2*A1+A30+A3*B3+14*A2*B2						[346]
C ₁₇ H ₃₆ O	9-heptadecanol						
	330.2	43.2	0	130.8	157.3	43.2	51.9
	Note: Authors report the sum of the fusion enthalpy plus all phase transitions above 298 K						
	2*A1+A30+A3*B3+14*A2*B2						[346]
C ₁₈ H ₁₂ O ₃	1,6-dimethylphenanthro[1,2-b]furan-10,11-dione						[568-73-0]
	495.4	22.09	0	44.6	59.3	22.1	29.4
	2*A14+3*A15+5*A19+A18*B18+A112+2*A114++2*A1+5*A10+A11+2*A12						[112]
C ₁₈ H ₁₃ ClN ₂ O ₃	2-cyano-6-methoxy-1(2 <i>H</i>)-quinolinecarboxylic acid, 4-chlorophenyl ester						
	374.2	22.35	0	59.7	65.3	22.4	24.4
	A14+3*A15+7*A10+3*A12+2*A19+2*A18+A16+A1+A32+A56+						
	A22*D22+A169						[274]
C ₁₈ H ₁₄ F ₄ N ₂ O ₄ S	Bicalutamide						
(I)	465.2	47.77	0	102.7	88.3	47.8	41.1
(II)	462.2	43.04	0	93.1	88.3	43.0	40.8
	7*A10+A11+4*A12+A60+A88+2*A4*B4+A2+A1+A30*D30+3*A25+A24+A56						[366]

C ₁₈ H ₁₄ N ₂ O ₂	1-benzyoyl-1,2-dihydro-6-methoxy-2-quinolinecarbonitrile						
396.0	23.11	0	58.4	69.5	23.1	27.5	
	A14+3*A15+8*A10+2*A12+2*A19+2*A18+A16+A146+A56+A1+A32					[274]	
C ₁₈ H ₁₄ N ₂ O ₃	2-cyano-6-methoxy-1(2 <i>H</i>)-quinolinecarboxylic acid, phenyl ester						
384.0	22.88	0	59.6	64.0	22.9	24.6	
	A14+3*A15+8*A10+2*A12+2*A19+2*A18+A16+A1+A32+A56+A169					[274]	
C ₁₈ H ₁₄ O ₃	1,2-dihydro-1,6-dimethylphenanthro[1,2- <i>b</i>]furan-10,11-dione						[87205-99-0]
490.3	22.22	0	45.3	47.7	22.2	23.4	
	2*A14+3*A15+5*A19+A16+A112+2*A114+2*A1+5*A10+A11+2*A12					[112]	
C ₁₈ H ₁₅ ClN ₂ O ₂ S	Etoricoxib						
407.1	30.43	0	74.8	84.6	30.4	34.4	
	9*A10+6*A12+A11+2*A1+2*A41+A88+A22*D22					[326]	
C ₁₈ H ₁₇ NO ₃	1-[(4-nitrophenyl)ethynyl]-4-butoxybenzene						
374.7	21.84	0	58.3	81.9	21.8	30.7	
	8*A10+4*A12+A50+3*A2+A1+2*A9+A32					[153]	
C ₁₈ H ₁₇ NO ₅	2-[[3-(3,4-dimethoxyphenyl)-1-oxo-2-propenyl]amino]benzoic acid (Tranilast)						
486.4	48.87	0	100.5	94.5	48.9	46.0	
	7*A10+5*A12+2*A1+2*A32+A60+A36*D36+A6*B6					[285]	
C ₁₈ H ₁₈ F ₃ N ₃ O ₃	3-{3,5-dimethyl-4-[3-(3-methylisoxazol-5-yl)propoxy]phenyl}-5-trifluoromethyl[1,2,4]oxodiazole (Pleconaril)						
(I) 336.5	29.3	0	87.1	111.0	29.3	37.4	
(II) 333.4	32.7	0	98.1	111.0	32.7	37.0	
	2*A14+4*A15+4*A19+A18+3*A118+2*A112+3*A1+3*A2+A4*B4+3*A25+A32+2*A10+2*A11+2*A12					[284]	
C ₁₈ H ₁₉ BrO	4-bromo-4'-(5-hexenyloxy)-1,1'-biphenyl						
308.2	13.8	44.78					
393.9	16.0	40.62	85.4	102.4	29.8	40.3	
	8*A10+4*A12+A32+4*A2+A21+A5+A6					[227]	
C ₁₈ H ₁₉ Cl ₂ NO ₄	(±) ethyl methyl 1,4-dihydro-2,6-dimethyl-4-(2,3-dichlorophenyl)-3,5-pyridine dicarboxylate (Felodipine)						
(I) 417.4	31.5	0	75.5	105.7	31.5	44.1	
(II) 405.7	26.7	0	65.8	105.7	26.7	42.9	
	Independent value from another reference						

412.3	34.8	0	84.4	105.7	34.8	43.6
	3*A10+2*A12+A11+4*A1+A2+A14+3*A15+4*A19+2*A38+A16+A121+2*A22*D22					[22, 418]
C ₁₈ H ₁₉ Cl ₂ NO ₄	(+) ethyl methyl 1,4-dihydro-2,6-dimethyl-4-(2,3-dichlorophenyl)-3,5-pyridine dicarboxylate (Felodipine)					
415.7	25.4	0	61.1	105.7	25.4	43.9
	3*A10+2*A12+A11+4*A1+A2+A14+3*A15+4*A19+2*A38+A16+A121+2*A22*D22					[22]
C ₁₈ H ₁₉ NO ₄	2-(4-nitrophenyl)-1-(4-butoxyphenyl)ethanone					
336.1	24.94	0	74.2	100.1	24.9	33.6
	A1+4*A2+8*A10+3*A12+A11+A32+A35+A50					[153]
C ₁₈ H ₂₀ N ₂ O ₄	diethyl 2,4,6,8-tetrahydro-4,8-ethanobenzo[1,2-c:4,5-c']dipyrrole-1,7-dicarboxylate					
439.3	18.2	0	41.4	100.9	18.2	44.3
	4*A14+2*A15+2*A16+6*A19+2*A18*B18+2*A38+2*A1+2*A2+2*A121					[107]
C ₁₈ H ₂₀ N ₂ O ₂	N,N'-bis(salicylaldehydo)tetramethylenediimine					
362.8	35.54	0	98.0	102.6	35.5	37.2
	8*A10+4*A12+4*A2+2*A6*B6+2*A42+2*A31					[253]
C ₁₈ H ₂₀ N ₂ O ₄	N-pentylthalidomide					
378.2	23.97	0	63.4	94.4	24.0	35.7
	4*A10+2*A14+5*A15+2*A19+2*A128+A16+A1+4*A2					[73]
C ₁₈ H ₂₀ OS	4'-(5-hexenyloxy)-[1,1'-biphenyl]-4-thiol					
358.4	11.6	32.37				
384.6	13.6	35.36	67.7	107.9	67.7	41.5
	8*A10+4*A12+A32+4*A2+A5+A6+A86					[227]
C ₁₈ H ₂₂ FNO ₃	(R)-deoxyephedrinium (S)-4'-fluoromandelate					
374.5	27.9	0	74.5	76.4	27.9	28.6
	10*A10+2*A11+A2+2*A1+A44+2*A3*B3+A180					[36]
C ₁₈ H ₂₂ FNO ₃	(R)-deoxyephedrinium (R)-4'-fluoromandelate					
369.2	26.6	0	72.1	74.2	26.6	27.4
	10*A10+2*A11+A2+2*A1+A44+2*A3*B3+A180					[36]
C ₁₈ H ₂₂ FNO ₄	(1R,2S)-ephedrinium (R)-4'-fluoromandelate					

	438.3	37.5	0	85.6	76.0	37.5	33.3
							[36]
	10*A10+2*A11+2*A1+A44+3*A3*B3+A180+A30*C30						
C ₁₈ H ₂₂ FNO ₄	(1R,2S)-ephedrinium (S)-4'-fluoromandelate						
	380.4	24.5	0	64.4	73.8	24.5	28.1
							[36]
	10*A10+2*A11+2*A1+A44+3*A3*B3+A180+A30*C30						
C ₁₈ H ₂₈ S ₈	2-[4,5-bis(propylthio)-1,3-dithiol-2-ylidene]-4,5-bis(propylthio)-1,3-dithiole						
	306.6	42.7	0	139.3	155.0	42.7	47.5
							[49]
	2*A14+4*A15+6*A19+4*A131+4*A84+4*A1+8*A2						
C ₁₈ H ₃₀	1,2,4,5-tetraisopropylbenzene						
	393.0	19.60	0	49.9	60.0	19.6	23.6
							[45]
	8*A1+2*A10+4*A12+4*A3						
C ₁₈ H ₃₆ O ₂	stearic acid						
	340.2	50.93	0	149.7	162.2	50.9	55.2
							[135]
	16*A2*B2+A36						
C ₁₈ H ₃₆ O ₂	methyl heptadecanoate						
	304.2	48.1	0	158.1	182.4	48.1	55.5
							[245]
	2*A1+15*A2*B2+A38						
C ₁₈ H ₃₇ NO	octadecanamide						
	298.7	2.2	7.36				
	379.7	54.8	144.32	151.7	194.3	57.0	73.7
							[391]
	A1+16*A2*B2+A61						
C ₁₈ H ₃₈ O	1-octadecanol						
	330.3	40.1	121.3				
	Independent values from another reference						
	329.5	26.5	80.42				
	330.3	40.1	121.40	201.8	177.4	66.6	58.5
							[208, 299]
	A1+17*A2*B2+A30						
C ₁₉ H ₁₃ NO	10-phenylacridin-9(10H)-one						
	550.0	38.9	0	70.7	63.3	38.9	34.8
							[180]
	13*A10+A12+A14+3*A15+4*A19+A114+A119						
C ₁₉ H ₁₆ ClNO	1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indole-acetic acid (Indomethacin)						
(I)	432.3	36.85	0	85.2	97.6	36.9	42.2

(II)	426.2	32.94	0	77.3	97.6	32.9	41.6
		Independent value from another reference					
	433.0	37.8	0	87.3	97.6	37.8	42.2
		A14+2*A15+4*A19+A146+2*A1+A2+7*A10+3*A12+A32+A36*D36+A22*D22					
							[238,240,418]
C ₁₉ H ₁₆ F ₈ O ₂		2,3-bis(trifluoromethyl)-4-methoxyphenyl- α,α -difluoro-4-n-propylbenzyl ether					
	301.4	21.3	0	70.7	88.7	21.3	26.7
		6*A10+4*A11+2*A12+3*A4*B4+6*A25+2*A26*B26+2*A1+2*A2+2*A32					
							[98]
C ₁₉ H ₁₆ O ₅		8-(hydroxymethyl)-6-phenyl-2-oxo-2H-1-benzopyran-3-carboxylic acid, ethyl ester					
	474.8	43.08	0	90.7	85.2	43.1	40.4
		A14+3*A15+3*A19+A18+A115+7*A10+A11+2*A12+A1+A2+A30*C30+A38					
							[129]
C ₁₉ H ₁₇ ClN ₂ O		Prazepam					
	419.0	27.69	0	66.1	86.2	27.7	36.1
		2*A14+4*A15+A16+A119+A118+3*A19+A2+8*A10+A12+A22*D22					
							[25]
C ₁₉ H ₁₈ N ₂ O ₃		1',3'-dihydro-1',3',3'-trimethyl-6-nitrospiro[2H-1-benzopyran-2,2'-(2H)-indole]					
	453.1	34.0	0	75.0	56.7	34.0	25.7
		2*A14+4*A15+4*A19+2*A18+2*A17+A119+A112+7*A10+A12+3*A1+A50					
							[201]
C ₁₉ H ₁₈ O ₃		6,7,8,9-tetrahydro-1,6,6-trimethylphenanthro[1,2-b]furan-10,11-dione					
							[568-72-9]
	486.9	30.46	0	62.6	64.6	30.5	31.5
	486.0	29.17	0	60.0	64.6	29.2	31.4
		3*A14+6*A15+7*A19+A17+2*A10+A18*B18+A112+2*A114+3*A1					
							[67,112]
C ₁₉ H ₁₈ O ₄		6,7,8,9-tetrahydro-6-(hydroxymethyl)1,6-dimethylphenanthro[1,2-b]-furan-10,11-dione					
							[17397-93-2]
	479.7	23.74	0	49.5	76.4	23.7	36.6
		3*A14+6*A15+7*A19+A17+2*A10+A18*B18+A112+2*A114+2*A1+A2+A30*D30					
							[67]
C ₁₉ H ₁₉ NO ₂		1-[(4-nitrophenyl)ethynyl]-4-pentylbenzene					
	342.7	21.46	0	62.6	84.3	21.5	28.9
		8*A10+4*A12+A50+4*A2+A1+2*A9					
							[153]
C ₁₉ H ₁₉ NO ₃		1-[(4-nitrophenyl)ethynyl]-4-pentyloxybenzene					
	359.9	33.56	0	93.3	89.0	33.6	32.0

		8*A10+4*A12+A50+4*A2+A1+2*A9+A32					[153]
C ₁₉ H ₁₉ NO ₄ S		ethyl 5-phenylsulfonyl-4,7-dihydro-4,7-ethano-2 <i>H</i> -isoindole-1-carboxylate					
	453.3	29.8	0	65.7	87.8	29.8	39.8
		3*A14+2*A15+2*A16+4*A19+A18+A18*B18+A121+A38+A88+A1+A2+5*A10+A12					[107]
C ₁₉ H ₂₀ O ₃		1,2,6,7,8,9-hexahydro-1,6,6-trimethylphenanthro[1,2- <i>b</i>]furan-10,11-dione [35825-57-11]					
	464.6	26.46	0	57.0	65.3	26.5	30.3
		3*A14+6*A15+6*A19+A17+A16+2*A10+A112+2*A114+3*A1					[112]
C ₁₉ H ₂₁ NO ₃		2-(4-nitrophenyl)-1-(4-pentylphenyl)ethanone					
	363.2	29.46	0	81.1	102.5	29.5	37.2
		A1+5*A2+8*A10+3*A12+A11+A35+A50					[153]
C ₁₉ H ₂₁ NO ₄		2-(4-nitrophenyl)-1-(4-pentyloxyphenyl)ethanone					
	353.4	27.07	0	76.6	107.2	27.1	37.9
		A1+5*A2+8*A10+3*A12+A11+A32+A35+A50					[153]
C ₁₉ H ₂₂ F ₈ O ₂		2,3- <i>bis</i> (trifluoromethyl)-4-methoxyphenyl- <i>trans</i> -4- <i>n</i> -propylcyclohexyl- α,α -difluoromethyl ether					
	314.7	21.4	0	68.00	100.5	21.4	31.6
		A14+3*A15+2*A16+2*A10+2*A11+2*A12+2*A1+3*A2+3*A4*B4+2*A26*C26+6*A25+2*A32					[98]
C ₁₉ H ₂₃ N ₃		N-methyl-N'-2,4-xylyl-N-(N-2,4-xylylformimidyl)formamidine (Amitraz)					
(I)	355.3	26.77	0	75.3	61.2	26.8	30.8
(II)	344.4	19.47	0	56.5	61.2	19.5	29.8
(III)	388.6	53.14	0	136.8	61.2 ^a	53.1	33.6
		5*A1+6*A10+2*A12+4*A11+2*A42+2*A6*B6+A43					[271]
C ₁₉ H ₂₆ FeO ₂ S ₃		1,9-dioxa-4,6,12-trithiacyclotetradecan-5-ylferrocene					
	367.1	40.0	0	109.0	107.2	40.0	39.3
		3*A14+15*A15+9*A18*B18+A19+A179+2*A112+3*A131+A16					[130]
C ₁₉ H ₂₆ FeO ₃ S ₂		1,9,12-trioxa-4,6-dithiacyclotetradecan-5-ylferrocene					
	349.7	32.1	0	91.8	105.5	32.1	36.9
		3*A14+15*A15+9*A18*B18+A19+A179+3*A112+2*A131+A16					[130]
C ₁₉ H ₂₇ NO ₄		(3 <i>R</i>)- β -cyano-3,4-dimethoxy- α,α -dimethyl- β -(1-methylethyl)benzenepropanoic					

	acid, ethyl ester						
386.4	8.82	0	22.8	88.6 ^a	8.8	34.2	
	7*A1+A2+A3+A4+A4*B4+3*A10+A11+2*A12+A56+2*A32+A38						[194]
C ₁₉ H ₃₇ AsO ₇	(R)-1,2-dicapryloxypropyl-3-arsonic acid						
347.7	41.8	0	120.2	137.3	41.8	47.7	
	2*A1+14*A2+2*A38+A3*B3+A181						[100]
C ₁₉ H ₃₇ AsO ₇	(S)-1,2-dicapryloxypropyl-3-arsonic acid						
346.7	37.66	0	108.6	137.3	37.66	47.6	
	2*A1+14*A2+2*A38+A3*B3+A181						[100]
C ₁₉ H ₃₈ O ₂	methyl stearate						
311.0	71.1	0	228.6	191.7	71.1	59.6	
	Independent value from another reference						
310.9	61.7	0	198.5	191.7	61.7	59.6	
	2*A1+A38+16*A2*B2						[193, 245]
C ₁₉ H ₄₀ O	1-nonadecanol						
333.9	43.3	0	129.7	186.7 ^a	43.3	62.3	
	Independent values from another reference						
329.7	29.1	88.26					
333.9	43.3	129.68	217.9	186.7	72.4	62.3	
	A1+18*A2*B2+A30						[208, 299]
C ₂₀ H ₄ Cl ₄ F ₁₃ NO ₂	4,5,6,7-dichloro-2-(4-n-tridecafluorohexylphenyl)isoindole-1,3-dione						
512.8	45.1	0	88.0	108.3	45.1	55.5	
	A14+2*A15+A129+2*A19+5*A12+4*A22*D22+A11+4*A10+6*A4*B4+3*A25+10*A26*B26						[117]
C ₂₀ H ₆ Cl ₂ F ₁₃ NO ₂	5,6-dichloro-2-(4-n-tridecafluorohexylphenyl)isoindole-1,3-dione						
459.6	40.7	0	88.6	105.7	40.7	48.6	
	A14+2*A15+A129+2*A19+3*A12+2*A22*D22+A11+6*A10+6*A4*B4+3*A25+10*A26*B26						[117]
C ₂₀ H ₆ Cl ₂ F ₁₃ NO ₂	4,7-dichloro-2-(4-n-tridecafluorohexylphenyl)isoindole-1,3-dione						
413.2	18.4	44.53					
417.2	19.9	47.70	92.2	105.7	38.3	44.1	
	A14+2*A15+A129+2*A19+3*A12+2*A22*D22+A11+6*A10+6*A4*B4+3*A25+10*A26*B26						[117]

C ₂₀ H ₁₀	corannulene						
542.3	17.3	0	31.9	33.0	17.3	17.9	
	10*A10+5*A12+5*A13						[31]
C ₂₀ H ₁₁ F ₁₄ N ₃	2,2,3,3,4,4,4-heptafluoro-N-[2,2,3,3,4,4,4-heptafluoro-1-(phenylamino)-butylidene]-N'-phenylbutanimidamide						
361.0	31.3	0	86.7	87.9	31.3	31.7	
	6*A4*B4+6*A25+8*A26*B26+2*A42+2*A7+10*A10+2*A12						[242]
C ₂₀ H ₁₂	benzo[k]fluoranthene						
490.6	27.5	0	56.1	35.6	27.5	17.5	
	12*A10+7*A12+A13						[247]
C ₂₀ H ₂₁ ClO ₄	2-[4-(4-chlorobenzoyl)phenoxy]-2-methylpropanoic acid, isopropyl ester (Fenofibrate)						
353.7	32.4	0	91.6	100.0	32.4	35.4	
	4*A1+8*A10+4*A12+A32+A35+A22*D22+A38+A3*B3+A4*B4						[81]
C ₂₀ H ₂₃ NO ₄	Naltrexone						
448.2	15.64	0	34.9	61.7	15.6	27.6	
	5*A14+2*A15+3*A16+2*A17+A114+A112+A119+2*A10+A12+A31+A30*D30+A2+3*A19						[235]
C ₂₀ H ₂₄ O ₂	19-norpregna-1,3,5(10)-trien-20-yne-3,17-diol (ethinyl estradiol)						
456.2	27.57	0	60.4	60.6	27.6	27.6	
	3*A14+4*A15+2*A17+3*A16+2*A19+A31+A1+A30*B30+A8+A9+3*A10+A12						[82]
C ₂₀ H ₂₃ N ₃ O ₉	N-[N-[[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethoxy]acetyl]-L-alanyl]-D-glutamic acid						[142489-47-2]
???	54.53	0			54.5		
	Compound not estimated						[34]
C ₂₀ H ₂₄ O ₂	7-methyl-3-(1-methylethyl)-8-(4-methyl-3-pentenyl)-1,2-naphthalenedione (Saprorthoquinone)						[102607-41-0]
369.2	23.09	0	62.5	79.2	23.1	29.2	
	A14+3*A15+3*A19+A18+2*A114+2*A10+2*A11+5*A1+2*A2+A3+A6+A7						[67]
C ₂₀ H ₂₄ O ₃	3-(acetyloxy)-estra-1,3,5(10)-trien-17-one						
399.0	15.0	0	37.59	69.7	15.0	27.1	

		3*A14+4*A15+3*A16+A17+2*A19+A114+2*A1+A38+3*A10+A12					[116]
C ₂₀ H ₂₆		4,4'-di- <i>tert</i> -butylbiphenyl					
	322.0	1.00	3.11				
	402.0	18.8	46.77	49.9	61.0	19.8	24.5
		8*A10+6*A1+2*A4+2*A12+2*A11					[28]
C ₂₀ H ₂₇ N ₅ O ₂		6-[4-(1-cyclohexyl-1 <i>H</i> -tetrazol-5-yl)butoxy]-3,4-dihydro-2(1 <i>H</i>)quinolinone (Cilostazol)					
(I)	432.0	4.72	0	10.93	110.9	4.72	47.9
(II)	408.8	3.89	0	9.52	110.9	3.89	45.3
(III)	419.0	4.28	0	10.21	110.9	4.28	46.5
		3*A14+8*A15+A16+3*A19+3*A118+A119+A124+A32+4*A2+3*A10+A12					[79]
		[Note: Reported fusion enthalpies are very small. Compound likely exhibits solid-solid transition(s) at lower temperature(s)]					
C ₂₀ H ₃₀		1,1'-biadamantane					
	336.3	1.15	3.42				
	509.6	1.30	2.55				
	561	70±10	124.78	130.8	50.4 ^a	72.5	28.3
		6*A14+2*A15+6*A16+2*A17					[421]
C ₂₀ H ₃₀ N ₄ O ₄		1,1'-(1,10-decanediyl) <i>bis</i> thymine					
	455.0	42.56	0	93.5	126.5	42.6	57.5
		10*A2 +2*A125+2A124+2*A14+6*A15+2*A1+2*A19+2*A18*B18					[110]
C ₂₀ H ₃₀ O ₂		17-methyl testosterone					
	439.0	27.8	0	63.3	57.9	27.8	25.4
		4*A14+5*A15+3*A17+3*A16+3*A1+A30*B30+A19+A18*B18+A114					[11]
C ₂₀ H ₄₀ O ₂		methyl nonadecanoate					
	313.2	63.8	0	203.7	201.0	63.8	63.0
		2*A1+A38+17*A2*B2					[245]
C ₂₀ H ₄₂		eicosane					
	311.6	69.03	0	221.5	202.6	69.0	63.1
		Independent values from another reference					
	310.2	69.8	0	225.0	202.6	69.8	62.9
		2*A1+18*A2*B2					[351, 446]
C ₂₀ H ₄₂ O		1-eicosanol					

336.6	43.6	0	129.5	196.0 ^a	43.6	66.0
Independent values from another reference						
335.5	28.4	84.65		196.0 ^a	28.4	65.8
336.6	43.6	129.53	214.2	196.0	72.0	66.0
A1+19*A2*B2+A30						[208, 299]
C ₂₁ H ₁₆ N ₂	2,4,5-triphenylimidazole					
505.7	0.73	1.44				
550.8	35.15	63.82	65.3	95.1	35.9	52.4
A14+2*A15+3*A19+A118+A121+15*A10+3*A12						[80]
C ₂₁ H ₂₀ Br ₈ O ₂	2,2-bis[3,5-dibromo-4-(2,3-dibromopropoxy)phenyl]propane					
???	39.63	0		123.9	39.63	
4*A10+6*A12+2*A11++2*A1+4*A2+2*A3*B3+A4+2*A32+8*A21						[40]
[Note: Solid sample was precipitated from a methanol-dichloromethane mixture. Abstract implies that the compound may have other crystal forms.]						
C ₂₁ H ₂₀ O ₁₂	2-(3,4-dihydroxyphenyl)-3-(β-D-glucofuranosyloxy)-5,7-dihydroxy-4H-1-benzopyran-4-one (Isoquercitrin)					
471.2	49.8	0	105.7	150.1	49.8	70.7
2*A14+5*A15+4*A19+A114+2*A112+4*A16+A2+A3*B3+A32+5*A12+5*A10+4*A31+4*A30*D30						[384]
C ₂₁ H ₂₁ N	4-methyl-N,N-bis(4-methylphenyl)benzenamine					
388.0	22.96	0	59.18	68.1	22.96	26.4
Independent value from another reference						
388.8	19.95	0	51.31	68.1	19.95	26.5
12*A10+3*A12+3*A11+3*A1+A43						[288, 349]
C ₂₁ H ₂₁ N	N-(3-methylphenyl)-N,N-bis(4-methylphenyl)amine					
329.9	21.71	0	65.81	68.1	21.71	22.5
3*A1+12*A10+3*A12+3*A11+A43						[349]
C ₂₁ H ₂₁ N	N,N-bis(3-methylphenyl)-N-(4-methylphenyl)amine					
362.7	26.39	0	72.76	68.1	26.39	24.7
3*A1+12*A10+3*A12+3*A11+A43						[349]
C ₂₁ H ₂₁ N	N,N,N-tris(3-methylphenyl)amine					
313.0	13.07	0	41.76	68.1	13.07	21.3
3*A1+12*A10+3*A12+3*A11+A43						[349]

C ₂₁ H ₂₅ NO	4-(1-methylheptyloxy)-4'-cyanobiphenyl							
(I)	287.8	20.8	0	72.27	112.5	20.8	32.4	
(II)	294.3	19.1	0	64.90	112.5	19.1	33.1	
		Independent values from another reference						
(I)	287.6	19.51	0	67.8	112.5	19.5	32.4	
(II)	294.3	17.07	0	58.0	112.5	17.1	33.1	
		8*A10+4*A12+2*A1+5*A2+A32+A3*B3+A56						[222,223]
C ₂₁ H ₂₆ O ₂	3-methoxy-19-norpregna-1,3,5(10)-trien-20-yn-17-ol (Mestranol)							
	424.1	34.55	0	81.5	62.6	34.6	26.5	
		4*A15+2*A19+3*A16+2*A17+3*A10+A12+2*A1+A32+A8+A9+A30*B30						[55]
C ₂₁ H ₂₆ O ₂	Cannabinol							
	352.2	17.0	0	48.3	75.9	17.0	26.7	
		A14+3*A15+4*A19+A17+A112+5*A10+2*A11+A124*A1+4*A2+A31						[55]
C ₂₁ H ₂₆ O ₃	3-(1-oxypoxy)-estra-1,3,5(10)-trien-17-one							
	409.0	23.0	0	56.2	75.0	23.0	30.7	
		3*A14+4*A15+2*A19+3*A16+A17+A114+3*A10+A12+2*A1+A2+A38						[116]
C ₂₁ H ₂₆ O ₄	4-{4-[4-(1,1-dimethylethyl)phenyl]-2-hydroxybutoxy}benzoic acid (Lifibrol)							
(I)	415.2	38.1	0	91.8	105.8	38.1	43.9	
(II)	408.2	49.1	0	120.3	105.8	49.1	43.2	
		8*A10+2*A12+2*A11+3*A2+3*A1+A4+A32+A3*B3+A30*C30+A36*D36						[90]
C ₂₁ H ₃₀ O ₂	Cannabidiol							
	340.7	28.4	0	83.4	110.2	28.4	37.5	
		A14+3*A15+2*A16+A18+A19+2*A11+2*A12+2*A10+A5+A7+3*A1+4*A2+2*A31						[224]
C ₂₁ H ₃₁ NO	6-dodecyloxyisoquinoline							
	321.3	38.93	0	121.2	133.2	38.9	42.8	
		6*A10+A41+3*A12+A1+11*A2+A32						[124]
C ₂₁ H ₃₅ N ₃ O ₂	N-palmitoylpyrazinamide							
	362.7	51.82	0	142.9	194.7	51.8	70.6	
		3*A10+A12+2*A41+A71+14*A2*B2+A1						[86]
C ₂₁ H ₃₆ N ₂ OS	N-[(3-methoxyphenyl)methyl]-N'-dodecylthiourea							
	361.7	52.87	0	146.2	169.6	52.9	61.4	
		A90+4*A10+A11+A12+A32+2*A1+11*A2*B2+A2						[262]

C ₂₁ H ₄₂ O ₂	methyl eicosanoate						
319.2	74.3	0	232.8	210.3	74.3	67.1	[245]
	2*A1+A38+18*A2*B2						
C ₂₂ H ₁₆	2-(biphen-4-yl)naphthalene						
489.5	25.10	0	51.3	73.4	25.1	35.9	[406]
	16*A10+6*A12						
C ₂₂ H ₁₆	2-(biphen-3-yl)naphthalene						
346.3	18.50	0	53.4	73.4	18.5	25.4	[406]
	16*A10+6*A12						
C ₂₂ H ₁₉ Br ₂ NO ₃	Deltamethrin						
372.2	26.73	0	71.8	96.5	26.7	35.9	[316]
	A14+A17+2*A16+2*A1+A6+A7+2*A21+A38+A3*B3+A56+2*A12+A11+9*A10+A32						
C ₂₂ H ₂₁ Cl ₃ N ₄ O	Rimonabant						
427.9	36.1	0	84.4	92.3	36.1	39.5	[418]
	2*A14+5*A15+A118+2*A119+3*A19+A60+5*A12+7*A10+A1+3*A22*D22						
C ₂₂ H ₂₃ NO ₃	Fenpropathrin						
322.5	18.57	0	57.6	82.2	18.6	26.5	[35]
	A14+A38+A3*B3+9*A10+A11+2*A12+A32+4*A1+2*A17+A16+A56						
C ₂₂ H ₂₅ NO ₃	2-(4-nitrophenyl)-1-[4-(<i>trans</i> -4-ethylcyclohexyl)phenyl]ethanone						
445.1	37.32	0	83.9	94.2	37.3	41.9	[153]
	A14+3*A15+2*A16+2*A11+2*A12+8*A10+2*A2+A1+A35+A50						
C ₂₂ H ₂₅ NO ₆	methyl Naltrexone-3-O-carbonate						
393.7	10.92	0	27.7	51.9	10.9	20.4	[235]
	5*A14+2*A15+3*A16+2*A17+A114+A112+A119+2*A10+A12+A30*D30+A2+3*A19+A149+A1						
C ₂₂ H ₂₇ NO ₂	Danazol						
501.8	35.5	0	70.8	62.6	35.5	31.4	[418]
	5*A14+5*A15+A18+A18*B18+3*A19+A118+A112+3*A17+3*A16+A30*C30+A8+A9+2*A1						
C ₂₂ H ₂₈ N ₂ O	N-phenyl-N-(1-phenethyl-4-piperidyl)propionanilide (Fentanyl)						

358.3	30.10	0	84.0	95.1	30.1	34.1
	A14+3*A15+A119+A59+3*A2+A1+10*A10+A11+A12+A16					[380]
C ₂₂ H ₂₈ O ₂	13-ethyl-17-hydroxy-11-methylene-18,19-dinorpregn-4-en-20-yn-3-one (Etonogestrel)					
472.2	31.15	0	66.0	65.7	31.2	31.0
	4*A14+4*A15+2*A19+A18+A114+A5+4*A16+2*A17+A8+A9+A30*B30+A1+A2					[82]
C ₂₂ H ₂₈ O ₃	3-[(1-oxobutyl)oxy]-estra-1,3,5(10)-trien-17-one					
381.0	22.0	0	57.7	82.1	22.0	31.3
	3*A14+4*A15+2*A19+3*A16+A17+3*A10+A12+A114+A38+2*A1+2*A2					[116]
C ₂₂ H ₃₃ N ₃ O ₂	Pyrimethanil decylate					
311.0	45.88	0	147.5	145.9	45.9	45.4
	3*A1+6*A10+2*A12+2*A11+2*A41+8*A2+A180					[342]
C ₂₂ H ₃₄ N ₄ O ₄	1,1'-(1,12-dodecanediyl)-bis-thymine					
462.0	43.95	0	95.1	140.7	43.95	65.0
	12*A2+2*A125+2*A124+2*A14+6*A15+2*A1+2*A19+2*A18*B18					[110]
C ₂₂ H ₄₄ O ₂	methyl heneicosanoate					
321.2	75.1	0	233.8	219.6	75.1	70.5
	2*A1+A38+19*A2*B2					[245]
C ₂₂ H ₄₅ NO	docosanamide					
383.3	63.3	0	165.1	231.2 ^a	63.3	88.6
	A1+20*A2*B2+A61					[391]
C ₂₃ H ₂₄ BNO ₂	4-benzyl-5,6-dimethyl-2,5-diphenyl-1,3-dioxo-4-aza-2-boracyclohexane					
408.2	13.00	0	31.9	44.0	13.0	18.0
	A14+3*A15+A172+A119+A16+A17+2*A1+A2+15*A10+2*A11+A12					[106]
C ₂₃ H ₂₇ NO ₃	2-(4-nitrophenyl)-1-[4-(<i>trans</i> -4-propylcyclohexyl)phenyl]ethanone					
436.5	38.87	0	89.1	108.4	38.9	47.3
	A14+3*A15+2*A16+8*A10+2*A11+2*A12+A35+A50+4*A2+A1					[153]
C ₂₃ H ₂₇ NO ₆	Ethyl Natrexone-3-O-carbonate					
404.2	18.99	0	46.8	59.0	19.0	23.8
	5*A14+2*A15+3*A16+2*A17+A114+A112+A119+2*A10+A12+A30*D30+A2+					

		3*A19+A149+A1+A2				[235]
C ₂₃ H ₂₈ ClN ₃ O ₅ S	Glyburide					
446.8	46.3	0	103.6	104.3	46.3	46.6
	A14+3*A15+A95+2*A60+7*A10+4*A12+A11+2*A2+A1+A32+A22*D22+A16					[418]
C ₂₃ H ₃₀ O ₃	3-[(1-oxopentyl)oxy]-estra-1,3,5(10)-trien-17-one					
398.0	25.0	0	62.81	89.2	25.0	35.5
	3*A14+4*A15+2*A19+3*A16+A17+3*A10+A12+A114+A38+2*A1+3*A2					[116]
C ₂₃ H ₃₀ O ₆	Prednisolone acetate					
515.0	42.3	0	82.14	84.8	42.3	43.7
	4*A14+5*A15+3*A17+4*A16+3*A1+2*A30*B30+A19+2*A18*B18+A18+A114+A35+A2+A38					[11]
C ₂₃ H ₃₂ O ₆	Hydrocortisone acetate					
480.0	53.64	0	111.8	89.5	53.64	42.9
	4*A14+5*A15+3*A17+4*A16+3*A1+2*A30*D30+A19+A18*B18+A114+A35+A2+A38					[11]
C ₂₃ H ₄₅ AsO ₇	(R)-1,2-dicapoxypropyl-3-arsonic acid					
358.3	68.20	0	190.3	200.9	68.20	72.0
	2*A1+16*A2*B2+2*A2+2*A38+A3*B3+A181					[100]
C ₂₃ H ₄₅ AsO ₇	(S)-1,2-dicapoxypropyl-3-arsonic acid					
358.5	54.39	0	151.7	200.9	54.39	72.0
	2*A1+16*A2*B2+2*A2+2*A38+A3*B3+A181					[100]
C ₂₃ H ₄₆ O ₂	methyl docosanoate					
327.2	83.5	0	255.2	228.9	83.5	74.9
	2*A1+A38+20*A2*B2					[245]
C ₂₄ H ₂₆ N ₂ O ₄	Carvedilol					
387.3	57.6	0	148.7	166.7	57.6	64.6
	A14+2*A15+11*A10+4*A19+A121+3*A12+A1+3*A31+4*A2+A44+A30*D30+A3*B3					[418]
C ₂₄ H ₂₇ NO ₅ S	Troglitazone					
412.4	48.8	0	118.3	118.1	48.8	48.7

C ₂₄ H ₃₇ N ₃ O	Pyrimethanil laurate						
321.5	67.24	0	209.1	160.1	67.2	51.5	
	3*A1+6*A10+2*A12+2*A11+2*A41+10*A2+A180						[255]
C ₂₄ H ₄₀ O ₃	5-(1,1-dimethylheptyl)-2-[(1R,2R,5R)-5-hydroxy-2-(3-hydroxypropyl)-cyclohexyl]phenol						
357.0	18.4	0	51.5	124.0 ^a	18.4	44.3	
	+A14+3*A15+3*A16+A31+2*A30*C30+3*A1+8*A2+A4+3*A10+2*A11+A12						[251]
C ₂₄ H ₄₀ N ₈ O ₄	dipyridamole						
(I) 442.8	44.05	0	99.5	150.5	44.1	66.6	
(II) 441.9	33.20	0	75.1		33.2	66.5	
	6*A12+4*A41+2*A14+6*A15+2*A119+2*A43+8*A2+4*A30*D30						[360]
C ₂₄ H ₅₀	tetracosane						
321.0	33.18	103.36					
324.1	59.31	183.00	286.4	239.8	92.49	77.7	
	22*A2*B2+2*A1						[439]
C ₂₄ H ₅₀ O	13-oxapentacosane						
303.8	4.60	15.14					
304.9	92.88	304.62	319.76	244.5 ^a	97.48	74.6	
	2*A1+22*A2*B2+A32						[189]
C ₂₅ H ₂₂ O ₁₀	silybin						
424.0	44.87	0	105.8	128.1	44.9	54.3	
	2*A14+6*A15+3*A112+4*A16+4*A19+A114+A1+A2+8*A10+4*A12+2*A11+A32+2*A30*D30+3*A31						[331, 341]
C ₂₅ H ₂₈ O ₃	estra-1,3,5(10)-triene-3,17-diol(17β), 3-benzoate						
464.1	41.75	0	90.0	84.2	41.8	39.1	
	3*A14+4*A15+2*A19+4*A16+A17+3*A10+A12+A1+A38+5*A10+A12+A30*B30						[55]
C ₂₅ H ₃₁ NO ₃	2-(4-nitrophenyl)-1-[4-[2-(<i>trans</i> -4-propylcyclohexyl)ethyl]phenyl]ethanone						
420.0	35.56	0	84.7	115.5	35.6	48.5	
	8*A10+2*A12+2*A11+A50+5*A2+A1+A35+A14+3*A15+2*A16						[153]
C ₂₅ H ₃₁ NO ₃	2-(4-nitrophenyl)-1-[4-(<i>trans</i> -4-pentylcyclohexyl)phenyl]ethanone						
415.8	34.48	0	82.9	115.5	34.5	48.0	

$A_{14}+2*A_{15}+4*A_{19}+A_{121}+12*A_{10}+4*A_{12}+2*A_{22}*D_{22}+2*A_{56}+2*A_{60}+2*A_7$ [132]

$C_{26}H_{29}NO$	Tamoxifen						
371.0	34.0	0	91.6	124.4	34.0	46.2	
	$14*A_{10}+4*A_{12}+3*A_2+3*A_1+A_{31}+2*A_7+A_{43}$						[418]
$C_{26}H_{32}O_6$	1,4,5,8-tetrakis(propoxy)-9,10-anthraquinone						
473.9	28.63	0	60.4	138.1 ^a	28.6	65.5	
	$A_{14}+3*A_{15}+4*A_{19}+2*A_{114}+4*A_{10}+4*A_{12}+4*A_{32}+4*A_1+8*A_2$						[93]
	[Note: The larger tetraalkoxy-derivatives show liquid crystalline behavior]						
$C_{26}H_{33}NO_3$	2-(4-nitrophenyl)-1-[4-[2-(<i>trans</i> -4-butylcyclohexyl)ethyl]phenyl]ethanone						
408.6	35.90	0	87.86	122.6	35.90	50.1	
	$8*A_{10}+2*A_{12}+2*A_{11}+A_{50}+6*A_2+A_1+A_{35}+A_{14}+3*A_{15}+2*A_{16}$						[153]
$C_{26}H_{34}O_4$	1,4,5,8-tetrapropoxyanthracene						
410.2	43.93	0	107.1	130.4	43.93	53.5	
	$4*A_1+8*A_2+4*A_{32}+6*A_{10}+8*A_{12}$						[93]
	[Note: Authors report only the total enthalpy of melting. Numerical value contains enthalpies for two solid-solid transitions that occur at 370.7 K and 385.5 K. Larger tetraalkoxy-derivatives show liquid crystalline behavior.]						
$C_{26}H_{36}O_3$	3-[(1-oxooctyl)oxy]-estra-1,3,5(10)-trien-17-one						
348.0	24.0	0	69.0	110.5	24.0	38.5	
	$3*A_{14}+4*A_{15}+2*A_{19}+3*A_{16}+A_{17}+3*A_{10}+A_{12}+A_{114}+A_{38}+2*A_1+6*A_2$						[116]
$C_{26}H_{38}O_2$	3 β -octyloxy-estra-1,3,5(10)-trien-17-one						
331.0	19.0	0	57.4	114.6	19.0	37.9	
	$3*A_{14}+4*A_{15}+2*A_{19}+3*A_{16}+A_{17}+3*A_{10}+A_{12}+A_{114}+A_{32}+2*A_1+7*A_2$						[116]
$C_{26}H_{40}O_2$	3-(octyloxy)-estra-1,3,5(10)-trien-17-ol						
338.0	21.0	0	62.1	111.9	21.0	37.8	
	$3*A_{14}+4*A_{15}+2*A_{19}+4*A_{16}+A_{17}+3*A_{10}+A_{12}+A_{32}+2*A_1+7*A_2+A_{30}*B_{30}$						[116]
$C_{26}H_{48}N_6O_9$	formamide deferoxamine						
430.8	92.93	0	215.7	215.7	92.9	92.9	
	$A_1+19*A_2+2*A_{60}+3*A_{30}*D_{30}+3*A_{59}+A_{162}$						[89]
$C_{26}H_{52}O_2$	methyl pentacosanoate						
332.2	92.0	0	276.94	256.8	92.0	85.3	
	$2*A_1+A_{38}+23*A_2*B_2$						[245]

C ₂₇ H ₁₉ NO	2-phenyl-5-(<i>p</i> -terphenyl-4-yl)oxazole					
504.2	42.0	0	83.3	103.0	42.0	51.9
	+A14+2*A15+A112+A118+A18*B18+2*A19+18*A10+6*A12					[123]
C ₂₇ H ₁₉ NO	2-(<i>p</i> -terphenyl-4-yl)-5-phenyloxazole					
485.2	37.0	0	76.26	103.0	37.0	50.0
	A14+2*A15+A112+A118+A18*B18+2*A19+18*A10+6*A12					[123]
C ₂₇ H ₃₀ O ₁₆	3-[[6-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4 <i>H</i> -1-benzopyran-4-one (Rutin)					
450.2	82.3	0	182.8	179.9	82.3	81.0
	3*A14+9*A15+A18*B18+3*A19+A112+A114+4*A10+6*A12+2*A32+A1+A2+4*A31+6*A30*D30+10*A16					[384]
C ₂₇ H ₃₅ NO ₃	2-(4-nitrophenyl)-1-[4-[2-(<i>trans</i> -4-pentylcyclohexyl)ethyl]phenyl]ethanone					
409.0	37.95	0	92.79	129.7	37.95	53.0
	8*A10+2*A12+2*A11+A50+7*A2+A1+A35+A14+3*A15+2*A16					[153]
C ₂₇ H ₃₈ O ₃	3-[(1-oxononyl)oxy]-estra-1,3,5(10)-trien-17-one					
337.0	24.0	0	71.2	117.7	24.0	39.6
	3*A14+4*A15+2*A19+3*A16+A17+3*A10+A12+A114+A38+2*A1+7*A2					[116]
C ₂₇ H ₄₆ O	5-cholesten-3 β -ol					
422.5	26.5	0	62.72	73.7	26.5	31.1
	4*A14+5*A15+5*A16+2*A17+A18+A19+2*A3+5*A1+3*A2+A30					[18]
C ₂₇ H ₄₆ O	cholesterol					
311.7	2.71	8.69				
423.2	21.11	49.88	58.6	73.7	23.8	31.1
	Independent value from another source					
423.2	25.10	0	59.3	73.7	25.1	31.1
	4*A14+5*A15+5*A16+2*A17+5*A1+3*A2+2*A3+A30+A19+A18					[225, 441]
C ₂₇ H ₄₈ N ₂ OS	N-[(3-methoxyphenyl)methyl]-N'-octadecylthiourea					
375.2	64.17	0	171.0	225.4	64.2	84.6
	A90+A2+17*A2*B2+2*A1+A32+4*A10+A11+A12					[262]
C ₂₇ H ₄₈ O	5 α -cholestan-3 β -ol					
413.5	22.6	0	54.7	72.9	22.6	30.1
	4*A14+5*A15+6*A16+2*A17+2*A3+5*A1+3*A2+A30					[18]

C ₂₇ H ₄₈ O	5β-cholestan-3α-ol					
385.8	15.8	0	41.0	72.9	15.8	28.1
	4*A14+5*A15+6*A16+2*A17+2*A3+5*A1+3*A2+A30					[18]
C ₂₇ H ₄₈ O	5β-cholestan-3β-ol					
373.8	16.1	0	43.1	72.9	16.1	27.3
	4*A14+5*A15+6*A16+2*A17+2*A3+5*A1+3*A2+A30					[19]
C ₂₇ H ₅₀ N ₆ O ₉	acetamide deferoxamine					
448.9	118.4	0	263.8	207.8	118.4	93.3
	2*A1+19*A2+2*A60+3*A30*D30+3*A59+A60					[89]
C ₂₇ H ₅₃ AsO ₇	(R)-1,2-dilauryloxypropyl-3-arsonic acid					
364.9	76.99	0	211.0	238.1	77.0	86.9
	2*A1+20*A2*B2+2*A2+2*A38+A3*B3+A181					[100]
C ₂₇ H ₅₃ AsO ₇	(S)-1,2-dilauryloxypropyl-3-arsonic acid					
363.3	65.69	0	180.8	238.1 ^a	65.69	86.5
	2*A1+20*A2*B2+2*A2+2*A38+A3*B3+A181					[100]
	The (R) and (S) enantiomers should have the same value unless they are polymorphs					
C ₂₇ H ₅₄ O ₂	methyl hexacosanoate					
336.2	101.3	0	301.31	266.1	101.3	85.9
	2*A1+A38+24*A2*B2					[245]
C ₂₈ H ₂₀ S	3-(<i>p</i> -terphenyl-4-yl)-5-phenylthiophene					
561.2	43.0	0	76.62	102.6	43.0	57.6
	18*A10+6*A12+A14+2*A15+A131+2*A19+A18*B18+A18					[123]
C ₂₈ H ₂₀ S	3-(<i>p</i> -terphenyl-4-yl)-4-phenylthiophene					
554.2	42.0	0	75.78	101.2	42.0	56.1
	18*A10+6*A12+A14+2*A15+A131+2*A19+2*A18*B18					[123]
C ₂₈ H ₂₀ S	2,5- <i>bis</i> (biphenyl-4-yl)thiophene					
595.2	39.0	0	65.52	104.1	39.0	62.0
	18*A10+6*A12+A14+2*A15+A131+2*A19+2*A18					[123]
C ₂₈ H ₂₄ O ₁₆ S ₄	4-sulfonato-calix[4]arene					
549.8	192.4	0	349.9		192.4	
	prediction not made					[339]

C ₂₈ H ₂₆ N ₄ O ₈	1,4- <i>bis</i> (3-phenylcarbamoyl-2-oxo-5-oxazolidin-5-ylmethoxy)benzene						
(I)	475.2	10.1	0	21.25		10.1	
(II)	502.2	5.1	0	10.15		5.1	
	prediction not made						[143]
C ₂₈ H ₄₀ O ₃	3-[(1-oxodecyl)oxy]-estra-1,3,5(10)-trien-17-one						
	344.0	29.0	0	84.3	121.7	29.0	41.9
	3*A14+4*A15+2*A19+3*A16+A17+3*A10+A12+A114+A32+2*A1+8*A2						[116]
C ₂₈ H ₃₁ FN ₄ O	Astemizole						
	447.6	51.1	0	114.2	105.1	51.1	47.0
	2*A14+5*A15+2*A119+A118+3*A19+12*A10+2*A12+2*A11+3*A2+A1+A32+A16+A44+A24						[418]
C ₂₈ H ₅₀ N ₆ O ₁₀ S	Methylsulfonamide Deferoxamine						
	416.0	117.8	0	283.2	212.9 ^a	117.8	88.6
	2*A1+19*A2+2*A60+3*A30*D30+3*A59+A95						[89]
C ₂₈ H ₅₂ N ₆ O ₉	Propylamide Deferoxamine						
	449.6	116.9	0	260.0	214.9	116.9	96.6
	2*A1+20*A2+2*A60+3*A30*D30+3*A59+A60						[89]
C ₂₈ H ₅₆ O ₂	methyl heptacosanoate						
	336.2	100.7	0	299.5	275.4	100.7	92.6
	2*A1+A38+25*A2*B2						[245]
C ₂₈ H ₅₈	octacosane						
	329.6	31.52	95.63				
	334.2	67.38	201.62	297.3	277.0	98.90	92.6
	26*A2*B2+2*A1						[439]
C ₂₈ H ₅₈ O	15-oxanonacosane						
	315.6	8.37	26.52				
	316.8	113.39	357.92	384.4	281.7	121.8	89.3
	2*A1+26*A2*B2+A32						[189]
C ₂₉ H ₂₆ BCl ₂ NO ₂	4-benzhydryl-2,5-di(4'-chlorophenyl)-4,5-dimethyl-1,3-dioxo-4-aza-2-boracyclohexane						
	453.2	23.96	0	52.9	57.1	24.0	25.9
	A14+3*A15+A172+A119+A16+A17+2*A1+A3*B3+18*A10+3*A11+						

3*A12+2*A22*D22 [106]

[Note: Sample may have experienced partial decomposition as authors report a mass decrease at melting.]

C₂₉H₂₈BNO₂ 4-benzhydryl-5,6-dimethyl-2,5-diphenyl-1,3-dioxo-4-aza-2-boracyclohexane
 431.2 28.43 0 65.9 54.5 28.4 23.5
 A14+3*A15+A172+A119+A16+A17+2*A1+A3*B3+20*A10+3*A11+A12 [106]

C₂₉H₄₂O₃ 3-[(1-oxoundecyl)oxy]-estra-1,3,5(10)-trien-17-one
 345.0 34.0 0 98.6 121.7 34.0 42.0
 3*A14+4*A15+2*A19+3*A16+A17+3*A10+A12+A114+A32+2*A1+8*A2 [116]

C₂₉H₄₄O₆Si₂4-[[1-oxo-11-(1,1,3,3-tetramethyldisiloxanyl)undecyl]oxy]benzoic acid,
 4-methoxyphenyl ester
 322.0 20.1 62.42
 331.0 5.4 16.31 78.7 25.5
 prediction not made [343]

C₂₉H₄₄O₆Si₂4-methoxybenzoic acid, 4-[[1-oxo-11-(1,1,3,3-tetramethyldisiloxanyl)undecyl]-
 oxy]phenyl ester
 324.0 24.3 75.00
 334.0 4.7 14.07 89.07 29.0
 prediction not made [343]

C₂₉H₅₁N₆O₁₁ Succinamide Deferoxamine
 436.2 101.0 0 231.5 234.6 101.0 102.3
 A1+21*A2+2*A60+3*A30*D30+3*A59+A60+A36*D36 [89]

C₂₉H₅₄N₆O₉ Butylamide Deferoxamine
 451.1 111.4 0 247.0 222.0 111.4 100.2
 2*A1+21*A2+2*A60+3*A30*D30+3*A59+A60 [89]

C₂₉H₅₈O₂ methyl octacosanoate
 340.2 109.7 0 322.46 284.7 109.7 96.9
 2*A1+A38+26*A2*B2 [245]

C₃₀H₂₂ 1,3-bis(biphenyl-4-yl)benzene
 548.2 55.0 0 100.3 102.8 55.0 56.4
 22*A10+8*A12 [123]

C₃₀H₂₂ 1-(*p*-terphenyl-4-yl)-3-phenylbenzene

	531.2	56.0	0	105.4	102.8	56.0	54.6
		22*A10+8*A12					[123]
C ₃₀ H ₄₄ O ₃		3-[(1-oxododecyl)oxy]-estra-1,3,5(10)-trien-17-one					
	342.0	31.0	0	90.6	128.8	31.0	44.1
		3*A14+4*A15+2*A19+3*A16+A17+3*A10+A12+A114+A32+2*A1+9*A2					[116]
C ₃₀ H ₄₆ F ₄ O ₂		cholesteryl 2,2,3,3-tetrafluoropropionate					
	422.6	28.6	0	67.7	102.9	28.6	43.5
		4*A14+5*A15+5*A16+2*A17+5*A1+3*A2+2*A3+A38+A19+A18+A4*B4+A3*B3+4*A26*B26					[142]
C ₃₀ H ₄₉ BrO ₂		cholesteryl α-bromopropionate					
	409.5	35.7	0	87.2	105.0	35.7	43.0
		4*A14+5*A15+5*A16+2*A17+6*A1+3*A2+2*A3+A38+A19+A18+A3*B3+A21					[142]
C ₃₀ H ₄₉ ClO ₂		cholesteryl α-chloropropionate					
	409.1	48.5	0	118.55	103.7	48.5	42.4
		4*A14+5*A15+5*A16+2*A17+6*A1+3*A2+2*A3+A38+A19+A18+A3*B3+A22*D22					[142]
C ₃₀ H ₅₆ N ₆ O ₉		Valeramide Deferoxamine					
	453.6	123.1	0	271.4	229.1	123.1	103.9
		2*A1+22*A2+2*A60+3*A30*D30+3*A59+A60					[89]
C ₃₀ H ₆₀		15-triacontene					
	324.2	30.96	95.50				
	325.2	49.79	153.11	248.51	269.0	80.75	87.5
		2*A1+2*A6+24*A2*B2					[189]
C ₃₁ H ₃₂ BNO ₂		4-benzhydryl-5,6-dimethyl-2,5-di(4'-methylphenyl)-1,3-dioxo-4-aza-2-boracyclohexane					
	453.2	32.48	0	71.67	55.7	32.48	25.2
		A14+3*A15+A172+A119+A16+A17+2*A1+A3*B3+18*A10+5*A11+A12+2*A1					[106]
C ₃₁ H ₅₂ O ₂		cholesteryl α-methylpropionate					
	400.7	25.2	0	62.9	105.1	25.2	42.1
		4*A14+5*A15+5*A16+2*A17+7*A1+3*A2+2*A3+A38+A19+A18+A3*B3					[142]
C ₃₁ H ₅₈ N ₆ O ₉		Caproylamide Deferoxamine					

	450.1	119.2	0	264.8	236.2	119.2	106.3
							[89]
C ₃₁ H ₆₁ AsO ₇							
	373.7	289.5	0	774.7	312.5 ^a	289.5	116.8
							[94]
C ₃₁ H ₆₁ AsO ₇							
	374.7	267.8	0	714.7	312.5 ^a	267.8	117.1
							[94]
C ₃₁ H ₆₂ O							
	356.4	117.1	0	328.6	300.2	117.1	107.0
							[297]
C ₃₂ H ₃₈ O ₆							
	334.2	49.27	0	147.4	157.2	49.3	52.5
							[115]
C ₃₂ H ₄₁ NO ₂							
	422.8	58.1	0	137.4	125.0	58.1	52.9
							[418]
C ₃₂ H ₅₂ N ₆ O ₉							
	453.8	107.0	0	235.8	219.7	107.0	99.7
							[89]
C ₃₂ H ₇₀ Si ₁₀							
	391.2	56.1	0	143.4	139.7	56.1	54.7
							[183]
C ₃₂ H ₆₆ O							
	323.2	10.46	32.36				
	324.7	116.73	359.50	391.86	318.9	127.19	103.6
							[189]
C ₃₃ H ₃₀ BNO ₂							
	454.2	25.48	0	56.1	54.3	25.5	24.6

	A14+3*A15+A172+A119+A16+A17+2*A1+A3*B3+22*A10+3*A11+3*A12	[106]
C ₃₃ H ₄₂ O ₄	17β-4-n-heptoxybenzoyloxy testosterone	
373.0	22.0 0 58.98 129.7 ^a 22.0	48.4
	4*A14+5*A15+4*A16+2*A17+A18*B18+A19+A114+A32+A38+4*A10+2*A12+6*A2+3*A1	[116]
C ₃₃ H ₅₄ N ₆ O ₉	Phenylacetamide Deferoxamine	
447.7	119.0 0 265.8 224.7 119.0	100.6
	A1+20*A2+2*A60+3*A30*D30+3*A59+A60+5*A10+A11	[89]
C ₃₃ H ₆₂ N ₆ O ₉	Octanoylamide Deferoxamine	
455.3	130.7 0 287.1 250.4 130.7	114.0
	2*A1+25*A2+2*A60+3*A30*D30+3*A59+A60	[89]
C ₃₄ H ₆₈	17-tetratriacontene	
332.8	33.47 100.57	
334.3	51.46 153.93 254.0 324.8 ^a 84.93	108.6
	2*A1+2*A6+30*A2*B2	[189]
C ₃₄ H ₇₀	tetratricontane	
342.8	0.41 1.20	
343.5	46.65 135.81	
346.1	95.64 276.34 413.4 332.8 ^a 142.7	115.2
	2*A1+32*A2*B2	[364]
C ₃₄ H ₇₆ Si ₁₁	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11-docosamethyl-1,11-diphenyl-undecasilane	
398.2	57.8 0 145.2 147.8 57.8	58.8
	11*A109+22*A1+10*A10+2*A12	[183]
C ₃₅ H ₃₇ N ₃	4-butylphenyl-[6-(4-butylphenyl)methyl-9-methyl-9 <i>H</i> -carbazol-3-ylmethylene]-amine	
460.2	29.6 0 64.3 151.9 ^a 29.6 69.9	
	A14+2*A15+4*A19+14*A10+4*A12+2*A11+2*A6*B6+2*A42+A119+3*A1+6*A2	[159]
C ₃₅ H ₃₇ N ₃ O ₂	4-butoxyphenyl-[6-(4-butoxyphenyl)methyl-9-methyl-9 <i>H</i> -carbazol-3-ylmethylene]amine	
475.2	34.4 0 72.4 161.3 ^a 34.4	
	A14+2*A15+4*A19+14*A10+4*A12+2*A11+2*A6*B6+2*A42+A119+3*A1+6*A2+2*A32	[159]

C ₃₅ H ₂₈ Cl ₂ N ₈ O ₄	Itraconazole						
438.6	69.9	0	159.4	130.2	69.9	57.1	
	4*A14+9*A15+3*A18*B18+3*A118+3*A119+A127+2*A112+A16+A17+A32+3*A2+2*A1+A3*B3+11*A10+6*A12+A11+2*A22*D22						[418]
C ₃₅ H ₅₀ N ₂ O ₈	2-methylacrylic acid 11-[4-(6,7,9,10,12,13,15,16-octahydro-5,8,11,14,17-pentaoxabenzocyclopentadecen-2-ylazo)phenoxy]undecyl ester						
379.7	48.7	0	128.26	236.1 ^a	48.7	89.7	
	A14+15*A15+5*A112+2*A19+7*A10+3*A12+2*A42+11*A2+A38+A5+A7+A1+A32						[303]
C ₃₅ H ₆₉ AsO ₇	(R)-1,2-dipalmitoyloxypropyl-3-arsonic acid						
377.3	250.6	0	664.2	312.5 ^a	250.6	117.9	
	28*A2*B2+2*A1+2*A38+2*A2+A3*B3+A181						[94]
C ₃₅ H ₆₉ AsO ₇	(S)-1,2-dipalmitoyloxypropyl-3-arsonic acid						
377.2	206.3	0	546.9	312.5 ^a	206.3	117.9	
	28*A2*B2+2*A1+2*A38+2*A2+A3*B3+A181						[94]
C ₃₆ H ₅₄ O ₁₂	benzene hexa-n-pentanoate						
173.1	8.8	50.6					
313.2	15.3	48.9					
349.9	1.4	4.0					
379.5	30.3	79.8	183.3	222	55.8	84.2	
	18*A2+6*A1+6*A38+6*A11						[51]
C ₃₆ H ₇₄	hexatricosane						
347.3	11.73	33.77					
348.3	24.72	70.97					
350.2	81.60	233.01	337.7	351.4	118.1	123.1	
	Independent value from another reference						
343.6	0.47	1.37					
346.8	15.02	43.31					
347.1	28.52	81.60					
349.2	102.51	293.56	419.8	351.4	143.5	122.7	
	2*A1+34*A2*B2						[351, 364]
C ₃₆ H ₇₄	18-methylpentatriacontane						
325.2	99.0	0	304.4	334.0	99.0	108.6	
	3*A1+A3+32*A2*B2						[322]

C ₃₆ H ₇₄ O	19-oxaheptatriacontane						
333.2	10.88	32.65					
335.3	105.86	315.72	348.4	356.1	116.7	119.4	
	2*A1+A32+34*A2*B2						[189]
C ₃₇ H ₄₈ N ₆ O ₅ S ₂	2,4,7,12-tetraazatriodecan-13-oic acid, 10-hydroxy-2-methyl-5-(1-methylethyl)-1-[2-(1-methylethyl)-4-thiazolyl]-3,6-dioxo-8,11-bis(phenylmethyl)-, 5-thiazolylmethyl ester (Ritonavir)						
395.5	57.9	0	146.4	175.7	57.9	69.5	
	4*A14+15*A15+A115+14*A16+3*A112+2*A17+2*A19+3*A32+13*A1+2*A2+2*A30*D30+A43						[81]
C ₃₇ H ₅₂ O ₄	3β-n-octyloxy-17β-butyloxybenzoxyloxy estradiol						
332.0	27.0	0	81.3	186.7 ^a	27.0	62.0	
	4*A14+5*A15+4*A16+A17+2*A19+7*A10+3*A12+A38+2*A32+10*A2+2*A1						[116]
C ₃₈ H ₇₆	19-octatriacontene						
321.0	7.53	23.46					
338.4	34.31	101.39					
340.8	66.53	195.22	320.07	362.0	108.37	123.4	
	2*A1+2*A6+34*A2*B2						[189]
C ₃₉ H ₄₅ N ₃ O ₂	4-hexyloxyphenyl-[6-(4-hexyloxyphenyl)methyl-9-methyl-9H-carbazol-3-yl-methylene]amine						
459.2	25.4	0	55.31	168.5 ^a	25.4	77.4	
	A14+2*A15+4*A19+14*A10+6*A12+2*A6*B6+2*A42+A119+3*A1+10*A2+2*A32						[159]
C ₃₉ H ₇₇ AsO ₇	(R)-1,2-distearoyloxypropyl-3-arsonic acid						
382.8	274.9	0	718.1	349.7 ^a	274.9	133.9	
	32*A2*B2+2*A1+2*A38+2*A2+A3*B3+A181						[94]
C ₃₉ H ₇₇ AsO ₇	(S)-1,2-distearoyloxypropyl-3-arsonic acid						
382.4	180.3	0	471.5	349.7 ^a	180.3	133.7	
	32*A2*B2+2*A1+2*A38+2*A2+A3*B3+A181						[94]
C ₃₈ H ₆₇ NO ₁₀	8,9-didehydro-N-demethyl-9-deoxo-4'',6,12-trideoxy-6,9-epoxy-N-Ethylerythromycin						[150785-53-8]
434.9	36.7	0	84.39	175.7 ^a	36.7	76.4	

4*A14+15*A15+A115+14*A16+3*A112+2*A17+2*A19+3*A32+13*A1+2*A2+
2*A30*D30+A43 [81]

C₃₈H₆₈S₈ 2-[4,5-*bis*(octylthio)-1,3-dithiol-2-ylidene]-4,5-*bis*(octylthio)-1,3-dithiole
94.3 0.16 1.70
215.8 4.92 22.80
322.5 89.3 276.9 301.4 297.0 94.38 95.8
2*A14+4*A15+4*A131+6*A19+4*A84+4*A1+28*A2 [49]

C₃₉H₇₈O 20-nonatricontanone
365.6 153.0 0 418.5 374.6 153.0 137.0
2*A1+A35+36*A2*B2 [297]

C₃₉H₈₀ 18-butylpentatriacontane
318.5 104.0 0 326.53 355.3 104.0 113.2
3*A1+3*A2+A3+32*A2*B2 [322]

C₄₀H₅₆ β-carotene
456.0 56.0 0 122.81 178.0 56.0 81.2
2*A14+6*A15+4*A19+2*A17+14*A6+4*A7+10*A1 [164]

C₄₀H₈₂ 20-methylnonatriacontane
331.4 120.0 0 362.10 371.2 120.0 123.0
3*A1+A3+36*A2*B2 [237]

Note: DSC curve showed no solid-solid phase transition in the temperature range of T = 300 K to T = 360 K

C₄₀H₈₂ tetracontane
345.0 2.51 7.28
347.7 8.60 24.73
354.6 143.94 405.92 437.9 388.6 155.05 137.8
2*A1+38*A2*B2 [364]

C₄₁H₄₄N₂O₉ 3,3'-di(N-cyclopropylmethyl)-4,5-epoxy-14-hydroxymorphinan-6-one-3-yl)
carbonate
490.6 17.5 0 35.67 75.6 17.5 37.1
10*A14+4*A15+6*A16+4*A17+2*A114+2*A112+2*A119+4*A10+2*A12+
2*A30*D30+2*A2+6*A19+A149 [250]

C₄₁H₇₆O₈ 3,5,5-trimethylhexanoic acid, 2,2-*bis*[[[(3,5,5-trimethyl-1-oxohexyl)oxy]-

	412.2	34.5	0	83.7	265.5 ^a	34.5	109.4
	A14+2*A15+4*A19+14*A10+4*A12+2*A11+2*A6*B6+2*A42+A119+3*A1+22*A2						[159]
C ₅₂ H ₃₄ O ₂							
	594.4	68.8	0	115.8	172.0	68.8	102.2
	1,4-bis(2,4,5-triphenylcyclopentadienone-3-yl)benzene 2*A14+4*A15+2*A114+8*A19+34*A10+8*A12						[252]
C ₅₄ H ₁₁₀							
	344.9	39.0	113.3				
	368.0	177.2	481.5	594.8	518.9	216.2	190.9
	tetrapentacontane 2*A1+52*A2*B2						[296]
C ₅₆ H ₄₈ O ₃₂ S ₄							
	543.1	350.6	0	645.6	96.5 ^a	350.6	52.4
	4-sulfonato-calix[8]arene 8*A145+A14+29*A15+8*A30*D30+24*A19+16*A10+8*A12						[339]
C ₅₇ H ₁₀₄ O ₆							
(I)	314.8	157.07	0	499.0	410.3	157.1	129.2
(II)	288.0	84.20	0	292.4		84.20	
	1,2,3-tri(<i>trans</i> -9-octadecenoyl)glycerol (Trielaidin) 3*A1+44*A2+A3*B3+3*A38+6*A6						[151]
C ₅₇ H ₁₁₀ O ₆							
(I)	345.9	197.6	0	571.26	526.7	197.6	182.2
(I)	346.0	195.8	0	565.90	526.7	195.8	182.2
(II)	327.3	129.1	0	394.44	526.7	129.1	172.4
(II)	327.3	114.1	0	348.61	526.7	114.1	172.4
	tristearin 3*A1+48*A2*B2+2*A2 +A3*B3+3*A38						[323]
C ₅₈ H ₈₅ N ₃							
	405.2	52.1	0	128.6	322.3 ^a	52.1	130.6
	4-hexadecylphenyl-[6-(4-hexadecylphenyl)methyl-9-methyl-9 <i>H</i> -carbazol-3-yl-methylene]amine A14+2*A15+4*A19+14*A10+4*A12+2*A11+2*A6*B6+2*A42+A119+3*A1+30*A2						[159]
C ₆₆ H ₁₀₉ NO ₄							
	333.2	61.87	0	185.7	374.6 ^a	61.9	124.8
	2,7-didodecyloxy-9-(3,5-didodecyloxyphenyl)carbazole A14+2*A15+4*A19+A119+9*A10+5*A12+4*A32+4*A1+40*A2						[97]
C ₇₂ H ₉₆ O ₄₈							
	505.7	74.37	0	147.1	359.5 ^a	74.4	181.8
	hexakis(2,3,4-tri- <i>O</i> -acetyl)- α -cyclodextrin						

		6*A14+18*A15+30*A16+6*A32+6*A112+6*A2+18*A38+18*A1					[362]
C ₈₄ H ₁₁₂ O ₅₆	heptakis(2,3,6-tri-O-acetyl)-β-cyclodextrin						
491.7	82.73	0	168.3	419.4 ^a	82.7	206.2	
	7*A14+21*A15+35*A16+7*A32+7*A112+7*A2+21*A38+21*A1					[362]	
C ₈₄ H ₁₄₄ O ₆	2,3,6,7,10,11-hexakis[[(2R,4R,6R)-2,4,6-trimethyloctyl]oxy]triphenylene						
141.2	38.0	269.12					
237.2	5.2	21.92	291.0	280.3	43.2	66.5	
	6*A10+12*A12+6*A32+24*A1+24*A2+18*A3					[172]	
C ₁₀₂ H ₁₈₀ O ₆	2,3,6,7,10,11-hexakis[[(2R,4R,6R,8R)-2,4,6,8-tetramethyldecyl]oxy]triphenylene						
139.2	23.4	168.10					
236.2	6.6	27.94	196.0	330.1 ^a	30.0	78.0	
	6*A10+12*A12+6*A32+30*A1+30*A2+24*A3					[172]	
NH ₇ S ₇	heptasulfur imide						
386.7	18.83	0	48.69		18.83		
	prediction not made					[85]	
N ₂ H ₅ NO ₃	α-hydrazinium nitrate						
	138.49 Joules/gram						
	prediction not made					[54]	
SeF ₂ O	selenium difluoride oxide						
288.0	8.08	0	28.06		8.08		
	prediction not made					[77]	

^a Not used in generating the statistics for both total phase change entropy and enthalpy

POLYMERS

Compound	T (K)	$(\Delta H_{pce})_n$	$(\Delta S_{pce})_n$	$(\Delta_0^{T_{fus}} S_{tpce})_n$ exp	$(\Delta_0^{T_{fus}} S_{tpce})_n$ calc	$(\Delta_0^{T_{fus}} H_{tpce})_n$ exp	$(\Delta_0^{T_{fus}} H_{tpce})_n$ calc
(C ₂ HClF ₃) _n							
	493.0	5.02	0	10.2	11.4	5.0	5.6
		A3*B3+A4*B4+2*A26*B26+A22*D22					[109]

$(C_2H_2F_2)_n$	poly(vinylidene fluoride)						
458.0	6.7	0	14.6	10.5	6.7	4.8	
	A2+A4*B4+2*A26						[109]
$(C_2H_2O_2)_n$	poly(glycolic acid)						
504.6	10.33	0	21.1	17.0	10.3	8.6	
	A38+A2*B2						[248]
$(C_2H_2S)_n$	poly(thioethylene)						
488.8	14.2	0	29.0	20.7	14.2	10.1	
	2*A2*B2+A84						[52,53]
$(C_2H_4S)_n$	poly(ethylene sulfide)						
489.0	14.0	0	28.6	20.7	14.0	10.1	
	2*A2*B2+A84						[109]
$(C_3H_4O)_n$	alternating ethylene and CO copolymer						
400.0	1.26	3.15					
507.0	7.79	15.36	18.51	23.2	9.05	11.8	
	2*A2*B2+A35						[128]
$(C_3H_4O_2)_n$	poly(lactic acid)						
480.0	6.55	0	13.65	15.5	6.55	7.4	
	A1+A3+A38						[229]
$(C_3H_5ClO)_n$	poly(epichlorohydrin)						
389.2	10.6	0	27.2	25.3	10.6	9.8	
	2*A2+A3*B3+A32+A22*B22						[57]
$(C_4H_6O)_n$	alternating propylene and CO copolymer						
364.0	8.3	0	22.8	19.5	8.3	7.1	
	A2+A3*B3+A1+A35						[141]
$(C_3H_6S)_n$	poly(trimethylene sulfide)						
368.0	10.4	0	28.3	19.5	10.4	11.0	
	3*A2*B2+A84						[109]
$(C_3H_6S)_n$	poly(trimethylene sulfide)						
363.2	10.46	0	28.3	30.0	10.5	11.9	
	3*A2*B2+A84						[348]

	346.5	23.4	0	67.6	60.5	23.4	21.0
							[75]
(C ₆ H ₁₂ S) _n							
	363.3	19.8	0	54.5	57.9	19.8	21.0
							[109]
(C ₇ H ₁₃ NO ₂) _n							
	445.0	32.0	0	71.9	63.6	32.0	28.3
							[204]
(C ₇ H ₁₄ N ₂ O) _n							
	573.0	13.9	0	24.3	47.7	13.9	27.3
							[109]
(C ₈ H ₁₂ O ₄) _n							
	405.2	18.9	0	46.7	66.8	18.9	27.1
							[108]
(C ₈ H ₁₂ O ₄) _n							
	326.2	21.7	0	66.4	66.8	21.7	21.8
							[101]
(C ₈ H ₁₄) _n							
	311.0	21.0	0	67.5	66.4	21.0	20.6
							[76]
							[52236-40-5]
(C ₈ H ₁₄) _n							
	350.0	23.8	0	68.00	66.4	23.8	23.2
							[109]
(C ₈ H ₁₅ NO) _n							
	458.0	30.0	0	65.5	66.6	30.0	30.5
							[109]
(C ₈ H ₁₆ O) _n							
	356.0	32.0	0	89.9	79.1	32.0	28.2
							[109]
(C ₉ H ₈ O) _n							
	538.0	12.8	0	23.8	31.4	12.8	16.9

							[99]
		$5 \cdot A_{10} + A_{12} + A_3 \cdot B_3 + A_2 + A_{35}$					
$(C_9H_{14}O_4)_n$	poly(ethylene pimelate)						
309.2	29.8	0	92.2	76.1	29.8	23.5	
	$5 \cdot A_2 \cdot B_2 + 2 \cdot A_2 + 2 \cdot A_{38}$					[101]	
$(C_{10}H_8O_5)_n$	poly(oxydiethylene terephthalate)						
337.0	44.0	0	130.6	63.1 ^a	44.0	21.3	
	$4 \cdot A_{10} + 2 \cdot A_{12} + 2 \cdot A_{38} + 4 \cdot A_2 + A_{32}$					[109]	
$(C_{10}H_{16}O_4)_n$	poly(ethylene suberate)						
336.2	26.2	0	77.9	85.4	26.2	28.7	
	$6 \cdot A_2 \cdot B_2 + 2 \cdot A_2 + 2 \cdot A_{38}$					[101]	
$(C_{10}H_{16}O_4S)_n$	poly(thiodiethylene adipate)						
334.2	23.7	0	70.8	74.3	23.7	24.8	
	$8 \cdot A_2 + 2 \cdot A_{38} + A_{84}$					[200]	
$(C_{10}H_{16}S)_n$	poly(3-hexylthiophene)						
(I) 496.3	2.86	0	5.75	53.5 ^a	2.86	26.6	
(II) 492.5	2.86	0	5.81	53.5 ^a	2.86	26.3	
	$5 \cdot A_2 + A_1 + A_{14} + 2 \cdot A_{15} + 2 \cdot A_{16} + A_{18} + A_{19} + A_{131}$					[337]	
$(C_{10}H_{18})_n$	<i>trans</i> polydecenamer						
353.0	32.9	0	93.2	85.0	32.9	26.6	
	$8 \cdot A_2 \cdot B_2 + 2 \cdot A_6$					[109]	
$(C_{10}H_{18}N_2O_2)_n$	poly(tetramethylene adipamide)						
623.0	41.6	0	66.8	77.4	41.6	48.2	
	$8 \cdot A_2 \cdot B_2 + 2 \cdot A_{60}$					[109]	
$(C_{10}H_{18}N_2O_4)_n$	poly(ethylene hexamethylenediurethane)						
443.0	42.0	0	94.81	90.0	42.0	39.9	
	Structure not estimated?					[109]	
$(C_{10}H_{18}N_2O_4)_n$	poly(1,4-diisocyanatobutane with 1,4-butanediol)						
474.0	41.9	0	88.4	90.0	41.9	42.7	
	$8 \cdot A_2 \cdot B_2 + 2 \cdot A_{69}$					[352]	
$(C_{11}H_{10}O_4)_n$	poly(trimethylene terephthalate)						
500.0	10.84	0	21.7	51.3 ^a	10.8	25.7	

$(C_{14}H_{24}N_2O_2)_n$	poly(piperazine sebacamide)	453.0	26.0	0	57.40	85.5	26.0	38.7
								[109]
								$+A_{14}+3*A_{15}+2*A_{146}+8*A_2*B_2$
$(C_{14}H_{24}O_4)_n$	poly(octamethylene adipate)	340.0	41.0	0	120.6	127.0	41.0	43.2
								[109]
								$12*A_2*B_2+2*A_{38}$
$(C_{15}H_{28}N_2O_4)_n$	poly(heptamethylene hexamethylenediurethane)	419.0	48.5	0	115.8	136.5	48.5	57.2
								[109]
								$13*A_2*B_2+2*A_{69}$
$(C_{16}H_{26}O_4)_n$	poly(octamethylene 4-octenedioate)	312.0	34.0	0	109.0	128.8	34.0	40.2
								[109]
								$8*A_2*B_2+4*A_2+2*A_6+2*A_{38}$
$(C_{16}H_{26}O_4)_n$	poly(decamethylene 3-hexenedioate)	339.0	36.0	0	106.2	133.2	36.0	45.2
								[109]
								$10*A_2*B_2+2*A_6+2*A_2+2*A_{38}$
$(C_{16}H_{30}N_2O_2)_n$	poly(hexamethylene sebacamide)	501.0	58.6	0	117.0	133.2	58.6	66.7
								[109]
								$14*A_2*B_2+2*A_{60}$
$(C_{16}H_{30}N_2O_4)_n$	poly(octamethylene hexamethylenediurethane)	430.0	55.2	0	128.4	145.8	55.2	62.7
								[109]
								$14*A_2*B_2+2*A_{69}$
$(C_{17}H_{16}N_2O_4)_n$	poly(ethylene 4,4'-methylenediphenylenediurethane)	512.0	48.0	0	93.8	61.9	48.0	31.7
								[109]
								$3*A_2+2*A_{69}+8*A_{10}+2*A_{11}+2*A_{12}$
$(C_{18}H_{24}O_4)_n$	poly(decamethylene terephthalate)	411.0	46.1	0	112.2	123.0	46.1	50.6
								[109]
								$10*A_2*B_2+2*A_{38}+4*A_{10}+2*A_{12}$
$(C_{18}H_{28}N_2O_4)_n$	poly(decamethylene hexamethylenediurethane)	427.0	56.5	0	132.3	164.4	56.5	70.2
								[109]
								$16*A_2*B_2+2*A_{69}$

	336.0	55.0	0	163.7	184.6	55.0	62.0
	14*A2*B2+4*A2+2*A6+2*A38						[109]
(C ₂₂ H ₄₀ O ₄) _n	poly(tetradecamethylene suberate)						
	355.0	66.0	0	185.9	201.4	66.0	71.5
	20*A2*B2+2*A38						[109]
(C ₂₄ H ₂₈ N ₂ O ₄) _n	poly(nonamethylene 4,4'-methylenediphenylenediurethane)						
	463.0	58.6	0	126.6	115.8	58.6	53.6
	10*A2+2*A69+8*A10+4*A12						[109]
(C ₂₅ H ₃₀ N ₂ O ₄) _n	poly(decamethylene 4,4'-methylenediphenylene diurethane)						
	465.0	69.0	0	148.4	122.9	69.0	57.1
	11*A2+2*A69+8*A10+4*A12						[109]
(C ₂₆ H ₅₀ N ₂ O ₂) _n	poly(tridecamethylene tridecanediamide)						
	456.0	97.2	0	213.2	226.2	97.2	103.2
	24*A2*B2+2*A60						[109]

DENDRIMERS

C ₄₀ H ₇₆ Si ₅	Si[CH ₂ CH ₂ CH ₂ Si(CH ₃)[CH ₂ CH=CH ₂] ₂] ₄						
	222.8	39.2	0	176	257.6 ^a	39.2	57.4
	A109+4*(A109+5*A2+2*A6+2*A5+A1)						[64]
C ₁₆₈ H ₃₆₄ O ₂₄ Si ₂₁	Si{CH ₂ CH ₂ CH ₂ Si(CH ₃)[CH ₂ CH ₂ CH ₂ Si(CH ₃) ₂ OSi(CH ₃) ₂ (CH ₂) ₁₀ -COOCH ₃] ₂] ₄						
	203.5	48.6	238				
	226.5	125.0	552	791	1127.6 ^a	173	255.4
	A109+4*(29*A2+11*A1+2*A38+5*A109+2*A32)						[47]

^a Not used in generating the statistics for both total phase change entropy and enthalpy

Table A2. References for Enthalpy of Fusion Data of Table A

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