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 ($\Delta_0^{T_{fus}} H_{tpce}$) in kJ·mol^{-1}, Phase Change Entropies (ΔS_{pce}), and Total Phase Change Entropies $\Delta_0^{T_{fus}} S_{tpce}$ in J·mol^{-1}·K^{-1} of Organic and Organometallic Compounds

T (K)	ΔH_{pce}	ΔS_{pce}	$\Delta_0^{T_{fus}} S_{tpce}$	$\Delta_0^{T_{fus}} S_{tpce}$	$\Delta_0^{T_{fus}} H_{tpce}$	$\Delta_0^{T_{fus}} H_{tpce}$
Compound	Calculation	exp	exp	calc	exp	calc
GeI_2	germanium diiodide					
701.2	33.3	0	47.5		33.3	
	prediction not made					[304]
$C_2HCl_2F_3$	1,1,1-trifluoro-2,2-dichloroethane					
145.7	5.51	0	37.8	39.2	5.51	5.7
	2*A22*D22+3*A25+A4*B4+A3*B3					[7]
$C_2H_3BrO_2$	bromoacetic acid					
319.2	13.9	0	43.5	40.8	13.9	13.0
	A21+A2+A36*B36					[104]
$C_2H_3ClO_2$	chloroacetic acid					
334.8	16.3	0	48.7	39.5	16.3	13.2
	A22*D22+A2+A36*B36					[104]
$C_2H_3IO_2$	iodoacetic acid					
355.1	15.5	0	43.7	42.7	15.5	15.2
	A29+A2+A36*B36					[104]
$C_2H_4N_2O_2$	oxamide					
356.2	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]
$C_2H_6N_2O$	1-methyl urea					
372.0	12.5	0	33.6	31.7	12.5	11.8
	A1+A67					[305]
$C_3H_2N_2$	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]
$C_3H_2N_2O_3$	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]
$C_3H_4N_4O_6$	1,3,3-trinitroazetidine					
373.8	29.0	0	77.6	48.6	29.0	18.2
	A14+A15+A120+2*A50+A17					[192]
$C_3H_4O_3$	ethylene carbonate					
311.2	13.0	0	41.8	42.1	13.0	13.1
	A14+2*A15+A116					[154]
$C_3H_4O_4$	malonic acid					
407.5	23.1	0	56.7	39.5	23.1	16.1
	A2+2*A36*B36					[215]
$C_3H_5NO_2$	dimethylene urethane					
360.0	17.3	0	48.1	56.1	17.3	20.2
	A14+2*A15+A154					[163]
C_3H_5NOS	2-mercapto-2-oxazoline					
370.0	15.9	0	43.0	43.4	15.9	16.1
	A14+2*A15+A163					[387]
C_3H_5NS	2-mercapto-2-thiazoline					
377.0	16.8	0	44.6	44.6	16.8	16.8
	A14+2*A15+A165					[387]

$C_3H_6N_2O$	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]
$C_3H_6N_2O_2$	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]
$C_3H_6O_3$	dimethyl carbonate					
220.1	Not reported					
278.2	11.58	41.62	28.1	42.2	11.58	7.8
	2*A1+A149					[154]
$C_3H_6S_3$	1,3,5-trithiane					
488.4	32.2	0	65.9	53.2	32.3	26.0
	A14+3*A15+3*A131					[10]
C_3H_7NO	propanamide					
352.6	12.9	0	36.6	52.6	12.9	18.5
	A1+A2+A61					[391]
C_3H_7NO	N,N-dimethylformamide					
212.9	8.95	0	42.0	42.1	8.95	9.0
	2*A1+A62					[400]
$C_3H_8N_2O$	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_3H_8O	1-propanol					
148.7	5.40	0	36.3	33.5	5.40	5.00
	A1+2*A2+A30					[187]
C_3H_9NO	3-amino-1-propanol					
284.1	16.9	0	59.5	67.0	16.9	19.0
	3*A2*B2+A45+A30*B30					[137]
$C_3H_{10}N_2$	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]

$C_4F_6N_2S$ 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]

$C_4H_2Cl_2S$ 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_4H_3ClS 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]

$C_4H_4N_2$ 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.

$C_4H_4N_2$ 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]

$C_4H_4N_2O_3$ 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]

$C_4H_6F_4O_2$ 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]

$C_4H_6O_3$ propylene carbonate

220.3	8.96	0	40. 7	45.0	8.96	9.9

2*A15+A14+A1+A16*B16+A116 [154]

$C_4H_6O_4$ 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_4H_7NOS 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]

$C_4H_7NO_2$ (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]

$C_4H_8N_2O_2$ succinamide

485.9	6.08	12.51		74.4		36.2

Decomposed prior to melting

2*A2+2*A61 [357]

$C_4H_8N_4O_4$ 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]

$C_4H_8OS_2$ 1,3-dithiane sulfoxide

361.9	22.6	0	62.45	62.5	22.6	22.6

A164+A14+A15*3+A131 [145]

$C_4H_8O_2S_2$ 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]

$C_4H_8O_2S_2$ 1,4-dithiane sulfone

474.2	26.0	0	54.8	45.2	26.9	21.4

A14+3*A15+A131+A134 [347]

$C_4H_8O_3$ ethyl methyl carbonate

219.4	11.24	0	51.2	35.2	11.24	7.7

2*A1+A2+A149 [154]

$C_4H_8O_3S$ 1,3-oxathiane sulfone

352.9	15.2	0	43.1	43.5	15.2	15.4
A14+3*A15+A112+A134						[347]

$C_4H_8O_3S$ 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_4H_9NO N,N-dimethylacetamide

254.2	10.20	0	40.1	41.6	10.20	10.6
3*A1+A59						[400]

C_4H_9NO butanamide

387.3	19.2	0	49.6	64.1	19.2	24.8
A1+2*A2*B2+A61						[391]

C_4H_9NO 2-methylpropanamide

400.1	19.2	0	48.0	53.3	19.2	21.3
2*A1+A3*B3+A61						[391]

$C_4H_{10}N_2O$ 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]

$C_4H_{10}O_2$ 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]

$C_4H_{10}O_2S_2$ meso 1,2-*bis*(methylsufinyl)ethane

446.7	34.31	0	76.8	65.4	34.31	29.2
2*A1+2*A2+2*A87						[119]

$C_4H_{10}O_2S_2$ racemic 1,2-*bis*(methylsufinyl)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]

$C_4H_{10}O_4$	erythritol					
391.2	38.9	0	99.4	83.6	38.9	32.7
2*A2+2*A3*B3+4*A30*D30						[324]
$C_4H_{10}O_4$	L-threitol					
361.8	29.1	0	80.43	83.6	29.1	30.2
2*A2+2*A3*B3+4*A30*D30						[324]
$C_4H_{12}N_2$	butane-1,4-diamine					
295.1	28.06	0	95.1	80.0	28.06	23.6
4*A2*B2+2*A45						[15]
$C_5H_2N_4O_6$	2,4,6-trinitropyridine					
436.2	22.0	0	50.4	56.3	22.0	24.6
2*A10+3*A12+A41+3*A50						[272]
$C_5H_4O_2S$	2-thiophenecarboxylic acid					
400.9	21.0	0	52.4	41.3	21.0	16.6
A14+2*A15+A131+2*A18+A18*B18+A19+A36*B36						[144]
$C_5H_4O_2S$	3-thiophenecarboxylic acid					
412.9	18.3	0	44.32	39.9	18.3	16.5
A14+2*A15+A131+A18+2*A18*B18+A19+A36*B36						[144]
$C_5H_4O_3$	2-furancarboxylic acid					
402.5	22.6	0	56.15	39.6	22.6	16.0
A14+2*A15+A112+2*A18+A18*B18+A19+A36*B36						[244]
$C_5H_4O_3$	3-furancarboxylic acid					
394.8	21.3	0	53.95	38.2	21.3	15.1
A14+2*A15+A112+A18+2*A18*B18+A19+A36*B36						[244]
$C_5H_5N_3O_2$	2-amino-5-nitropyridine					
461.4	29.2	0 +	63.29	57.2	29.2	26.4
3*A10+2*A12+A45+A50+A41						[427]
$C_5H_6N_2$	glutaronitrile					
242.0	12.03	0	49.71	63.3	12.03	15.3
2*A56+3*A2*B2						[402]
$C_5H_6O_5$	2-ketoglutaric acid					

388.7	28.59	0	73.55	62.4	28.59	24.2
2*A2+A36+A35+A36*B36						[329]

$C_5H_8F_4N_4O_2$ 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]

$C_5H_8N_4O_6$ 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]

$C_5H_8O_4$ 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]

$C_5H_{10}N_2O_2$ glutaramide

453.9	38.4	0	84.6	83.7	38.4	38.0
3*A2*B2+2*A61						[357]

$C_5H_{10}O_3$ diethyl carbonate

198.2	9.24	0	46.6	42.3	9.24	8.4
2*A1+2*A2+A149						[154]

$C_5H_{11}NO$ 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]

$C_5H_{11}NO$ 2,2-dimethylpropanamide

425.4	24.1	0	56.7	57.7	24.1	24.6
3*A1+A4*B4+A61						[391]

$C_5H_{12}N_2O$ 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]

$C_5H_{12}O$	1-pentanol					
195.6	10.51	0	53.7	56.5	10.5	11.1
A1+4*A2*B2+A30						[187]
$C_5H_{12}O$	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]
$C_5H_{12}O$	1,1-dimethyl-1-propanol (*tert*-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]						
$C_5H_{12}O$	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]
$C_5H_{12}O_5$	xylitol					
369.0	33.26	0	90.1	96.0	33.26	35.4
2*A2+3*A3*B3+5*A30*D30						[429]
$C_5H_{14}N_2$	pentane-1,5-diamine					
285.0	29.82	0	104.6	89.3	29.82	25.5
5*A2*B2+2*A45						[15]
C_6Br_6	hexabromobenzene					
598.8	24.6	0	41.1	60.0	24.6	35.9
6*A12+6*A21						[203]
$C_6N_8O_8$	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_6HBr_5O pentabromophenol

469.8 27.6 0 58.75 62.8 27.6 29.5

6*A12+A31+5*A21 [300]

$C_6H_2Br_4$ 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]

$C_6H_2N_4$ 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]

$C_6H_2N_4O_6$ 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]

$C_6H_3Br_3$ 1,2,4-tribromobenzene

317.0 17.9 0 56.5 52.2 17.9 16.5

3*A10+3*A12+3*A21 [203]

$C_6H_3Br_3$ 1,3,5-tribromobenzene

395.0 21.72 0 55.0 52.2 21.72 20.6

3*A10+3*A12+3*A21 [280]

$C_6H_3Br_3O$ 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]

$C_6H_3Cl_2NO_2$ 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]

$C_6H_3Cl_3$ 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]

$C_6H_3Cl_4N$ 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]

$C_6H_4Br_2$	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]
$C_6H_4Br_3N$	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_6H_4ClF	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]
$C_6H_4ClNO_2$	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]
$C_6H_4ClNO_2$	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]
$C_6H_4ClNO_2$	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]
$C_6H_4ClNO_3$	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]
$C_6H_4ClNO_3$	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]

$C_6H_4ClNO_3$	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]
$C_6H_4Cl_2$	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]
$C_6H_4Cl_2N_2O_2$	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]						
$C_6H_4N_2O_4$	1,3-dinitrobenzene					
360.4	19.68	0	54.6	50.0	19.68	18.0
4*A10+2*A12+2*A50						[157]
$C_6H_4N_2O_4$	1,4-dinitrobenzene					
446.0	17.58	0	39.4	50.0	17.58	22.3
4*A10+2*A12 +2*A50						[157]
$C_6H_4N_2O_5$	2,3-dinitrophenol					
419.0	22.67	0	54.1	62.9	22.67	26.4
3*A10+2*A12+2*A50+A31						[157]
$C_6H_4N_2O_5$	2,4-dinitrophenol					
383.2	26.19	0	68.4	62.9	26.19	24.1
3*A10+2*A12+2*A50+A31						[157]
$C_6H_4N_2O_5$	2,6-dinitrophenol					
329.0	22.91	0	69.6	62.9	22.91	20.7
3*A10+2*A12+2*A50+A31						[157]
$C_6H_4O_2$	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]
$C_6H_5Br_2N$	2,4-dibromoaniline					

351.4	21.37	0	60.8	56.1	21.37	19.7
	3*A10+3*A12+A45+2*A21					[371]
$C_6H_5Br_2N$	2,5-dibromoaniline					
328.1	20.47	0	62.4	56.1	20.47	18.4
	3*A10+3*A12+A45+2*A21					[371]
$C_6H_5Br_2N$	2,6-dibromoaniline					
355.5	21.79	0	61.3	56.1	21.79	19.9
	3*A10+3*A12+A45+2*A21					[371]
C_6H_5BrO	4-bromophenol					
338.2	17.6	0	52.0	52.4	17.6	17.7
	A21+4*A10+2*A12+A31					[300]
$C_6H_5Cl_2N$	3,4-dichloroaniline					
344.5	21.69	0	63.0	53.5	21.69	18.4
	3*A10+3*A12+A45+2*A22*D22					[147]
$C_6H_5NO_2$	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
	4*A10+A12+A41+A36*B36					[269, 443]
$C_6H_5NO_3$	2-nitrophenol					
316.3	17.05	0	53.9	52.6	17.05	16.6
	4*A10+2*A12+A50+A31					[157]
$C_6H_5NO_3$	3-nitrophenol					
369.0	18.06	0	48.94	52.6	18.06	19.4
	4*A10+2*A12+A50+A31					[157]
$C_6H_5NO_3$	4-nitrophenol					
386.4	11.00	0	28.47	52.6	11.00	20.3
	4*A10+2*A12+A50+A31					[157]
$C_6H_5NO_3$	(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_6H_6BrN		2-bromoaniline					
	304.1	16.14	0	53.08	53.5	16.14	16.3
	4*A10+2*A12+A45+A21						[371]
C_6H_6BrN		4-bromoaniline					
	336.0	16.75	0	49.85	53.5	16.75	18.0
	4*A10+2*A12+A45+A21						[371]
C_6H_6ClN		2-chloroaniline					
	269.2	12.38	0	45.99	52.2	12.38	14.1
	4*A10+2*A12+A45+A22*D22						[385]
C_6H_6ClN		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_6H_6IN		2-iodoaniline					
	329.6	19.38	0	58.80	55.4	19.38	18.3
	4*A10+2*A12+A45+A29						[358]
C_6H_6IN		4-iodoaniline					
	336.0	16.94	0	50.42	55.4	16.94	18.6
	4*A10+2*A12+A45+A29						[358]
$C_6H_6N_2O$		2-pyridinealdoxime					
	388.0	19.98	0	51.50	51.9	19.98	20.1
	4*A10+A12+A41+A53+A6						[404]
$C_6H_6N_2O$		nicotinamide					
	401.6	25.50	0	63.50	60.9	25.50	24.5
	4*A10+A12+A41+A61						[437]
$C_6H_6N_4O_4$		(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_6H_7NO	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_6H_7NO	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_6H_7NO	4-aminophenol						
455.2	23.8	0	52.3	56.3	23.8	25.6	
4*A10+2*A12+A31+A45							[48]
C_6H_7NO	4-pyridinemethanol						
325.2	11.78	0	36.22	55.7	11.78	18.1	
4*A10+A11+A30*B30+A41+A2							[318]
$C_6H_7NO_2S$	benzenesulfonamide						
425.8	25.2	0	59.11	54.7	25.17	23.3	
5*A10+A12+A96							[292]
$C_6H_8F_8N_4$	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]
$C_6H_8N_2$	adiponitrile						
275.0	18.0	0	65.5	72.6	18.0	20.0	
4*A2*B2+2*A56							[402]
$C_6H_8N_2O_2$	1,4-diisocyanoatobutane						
231.2	20.8	0	89.79	83.4	20.8	19.3	
4*A2*B2+2*A58							[328]
$C_6H_8N_2O_2S$	sulfanilamide						
435.4	23.3	0	53.5	61.2	23.3	26.6	
4*A10+2*A12+A45+A96							[168]
$C_6H_8N_4O_8$	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							
$C_6H_9N_3O_2$	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]
$C_6H_9N_3O_3$	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]
$C_6H_9N_3O_3$	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]
$C_6H_{10}O_4$	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]
$C_6H_{10}O_6$	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]
$C_6H_{10}O_6$	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]
$C_6H_{10}O_6$	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]
$C_6H_{10}O_6$	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]
$C_6H_{10}O_6$	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]

$C_6H_{11}NO$ caprolactam

342.2	16.2	0	47.2	50.9	16.2	17.4
A14+4*A15+A124						[393]

$C_6H_{11}NO$ 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]

$C_6H_{11}NO_2$ 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.]

$C_6H_{12}N_2OS$ N,N,N',N'-tetramethylmonothiooxamide

350.2	17.0	0	48.5	45.7	17.0	16.0
4*A1+A59+A175						[27]

$C_6H_{12}N_2O_2$ N,N,N',N'-tetramethyloxamide

352.2	18.0	0	51.11	48.0	18.0	16.9
4*A1+2*A59						[27]

$C_6H_{12}N_2O_2$ 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]

$C_6H_{12}N_2O_4$ 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]

$C_6H_{12}N_2S_2$ N,N,N',N'-tetramethyldithiooxamide

409.2	21.0	0	51.32	43.4	21.0	17.8
4*A1+2*A175						[27]

$C_6H_{12}O_2$ *cis* 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]
$C_6H_{12}O_2$	*trans* 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]
$C_6H_{12}S_3$	1,4,7-trithiacyclononane					
354.2	29.0	0	81.9	64.3	29.0	22.8
A14+6*A15+3*A131						[1]
$C_6H_{13}NO$	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]
$C_6H_{14}N_2$	*trans*-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]
$C_6H_{14}N_2O$	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]
$C_6H_{14}O$	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]
$C_6H_{14}O_2$	2,2-dimethoxybutane					
174.0	9.32	0	53.56	64.0	9.32	11.1
4*A1+A2+A4*B4+2*A32						[58]
$C_6H_{14}O_2$	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]

$C_6H_{14}O_2$	1,6-hexanediol					
316.0	25.5	0	80.70	91.1	25.5	28.8
2*A30*B30+6*A2*B2						[321]
$C_6H_{14}O_3$	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]
$C_6H_{14}O_6$	sorbitol					
369.2	30.35	0	82.20	108.5	30.35	40.0
2*A2+4*A3*B3+6*A30*D30						[435]
$C_6H_{16}N_2$	hexane-1,6-diamine					
312.3	40.21	0	128.8	98.6	40.21	30.8
6*A2*B2+2*A45						[15]
$C_6H_{18}AsN_3$	*tris*(dimethylamino)arsine					
222.6	13.3	0	59.79	42.1	13.31	9.4
6*A1+3*A43+A98						[12]
$C_7H_4Cl_2O$	2,4-dichlorobenzaldeyde					
347.2	20.47	0	59.0	53.6	20.5	18.6
3*A10+3*A12+A34+2*A22*D22						[185]
$C_7H_4N_2O_2$	2-nitrobenzonitrile					
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]
$C_7H_4N_2O_2$	3-nitrobenzonitrile					
389.7	20.49	0	52.6	50.0	20.5	19.5
4*A10+2*A12+A50+A56						[14]
$C_7H_4N_2O_2$	4-nitrobenzonitrile					
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]

$C_7H_4N_2O_5$	2,4-dinitrobenzaldehyde					
344.9	21.18	0	61.4	56.6	21.2	19.5
	3*A10+3*A12+A34+2*A50					[267]
$C_7H_5BrO_2$	2-bromobenzoic acid					
421.6	24.83	0	58.9	48.3	24.8	20.4
	4*A10+A36*B36+2*A12+A21					[265]
$C_7H_5BrO_2$	3-bromobenzoic acid					
430.1	24.91	0	57.9	48.3	24.9	20.8
	4*A10+A36*B36+2*A12+A21					[265]
$C_7H_5BrO_2$	4-bromobenzoic acid					
526.3	30.87	0	58.7	48.3	30.9	25.4
	4*A10+A36*B36+2*A12+A21					[265]
$C_7H_5ClO_2$	2-chlorobenzoic acid					
414.0	25.25	0	61.0	47.0	25.3	19.5
	4*A10+A36*B36+2*A12+A22*D22					[265]
$C_7H_5ClO_2$	3-chlorobenzoic acid					
427.9	23.67	0	55.32	47.0	23.7	20.1
	4*A10+A36*B36+2*A12+A22*D22					[265]
$C_7H_5ClO_2$	4-chlorobenzoic acid					
512.5	30.91	0	60.31	47.0	30.91	24.1
	4*A10+A36*B36+2*A12+A22*D22					[265]
C_7H_5NOS	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
	A14+2*A15+4*A10+2*A19+A163					[387, 407]
$C_7H_5NO_3S$	1,1-dioxo-1,2-benzisothiazol-3(2*H*)-one (Saccharin)					
500.7	29.89	0	59.7	59.7	29.9	29.9
	4*A10+A14+2*A15+2*A19+A166					[292]
$C_7H_5NO_4$	5-nitro-1,3-benzodioxole					
420.2	28.20	0	67.1	51	28.2	21.4
	A14+2*A15+2*A112+2*A19+3*A10+A12+A50					[396]

$C_7H_5NS_2$	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]
$C_7H_6Cl_2O$	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]
$C_7H_6Cl_2O$	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]
$C_7H_6N_2$	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]
$C_7H_6N_2S$	2-mercaptobenzimidazole					
589.4	24.11	0	40.9	40.9	24.1	24.1
A14+2*A15+4*A10+2*A19+ A168						[407]
$C_7H_6O_2$	4-hydroxybenzaldehyde					
390.8	21.6	0	55.4	56.4	21.6	22.0
4*A10+2*A12+A31+A34						[440]
$C_7H_6O_3$	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]
$C_7H_6O_3$	3-hydroxobenzoic acid					
476.4	36.5	0	76.62	51.1	36.5	24.4
4*A10+2*A12+A31+A36*B36						[327]
$C_7H_6O_3$	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
4*A10+2*A12+A31+A36*B36						[2, 355]

$C_7H_6O_3$ 5-hydroxy-1,3-benzodioxole (Sesamol)

337.7	16.96	0	50.22	53.6	16.96	18.1
A14+2*A15+3*A10+A12+A31+2*A19+2*A112						[177]

$C_7H_7ClN_2O_2$ N-methyl-N-(4-chlorophenyl)nitramine

323.4	19.5	0	60.3	58.7	19.5	19.0
A1+4*A10+2*A12+A22*D22+A51+A47						[127]

$C_7H_7NO_2$ 2-hydroxybenzamide (salicylamide)

411.9	29.0	0	70.41	62.8	29.0	25.9
4*A10+2*A12+A31+A61						[365]

$C_7H_7NO_2$ 3-aminobenzoic acid

445.7	33.7	0	75.61	52.2	33.7	23.3
4*A10+2*A12+A36*B36+A45						[48]

$C_7H_7NO_2$ 4-aminobenzoic acid

459.2	24.5	0	53.35	52.2	24.5	24.0
Independent values from another reference						
355.2	2.06	5.80				
458.7	22.62	49.31	55.11	52.2	24.68	24.0
4*A10+2*A12+A36*B36+A45						[48, 294]

$C_7H_7NO_2$ phenyl carbamate

(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
5*A10+A12+A70							[434]

$C_7H_7NO_3$ 4-aminosalicylic acid

406.2	47.9	0	117.9	71.6	47.9	29.1
3*A10+3*A12+A45+A36*D36+A31						[48]

$C_7H_7NO_3$ 5-aminosalicylic acid

543.2	67.2	0	123.7	71.6	67.2	38.9
3*A10+3*A12+A45+A36*D36+A31						[48]

$C_7H_7NO_4$ 2-methoxy-4-nitrophenol

374.4	21.69	0	57.93	60.0	21.69	22.5

	3*A10+3*A12+A50+A31+A1+A32					[209]
$C_7H_7NO_4$	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]
$C_7H_7NO_4$	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]
$C_7H_7N_3O_4$	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]
$C_7H_7N_3O_4$	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_7H_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_7H_8O	2-methylphenol					
305.4	14.8	0	48.5	50.4	14.8	15.4
	A31+A1+A12+4*A10+A11					[420]
C_7H_8O	3-methylphenol					
282.3	8.9	0	31.5	50.4	6.9	14.2
	A31+A1+A12+4*A10+A11					[420]
C_7H_8O	4-methylphenol					
308.8	12.6	0	40.8	50.4	12.6	15.6
	A31+A1+A12+4*A10+A11					[420]
$C_7H_8O_2$	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]
$C_7H_{10}ClN_3O_3$	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]

$C_7H_{10}N_2$ pimelonitrile

241.7	15.0	0	62.1	81.9	15.0	19.8

5*A2*B2+2*A56 [402]

$C_7H_{10}N_2$ 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]

C_7H_{12} norbornane

360.8	4.45	0	12.3	41.1	4.45	14.8

2*A14+A15+2*A16 [188]

$C_7H_{12}O_2$ cyclohexylcarboxylic acid

301.9	9.20	0	30.5	43.2	9.2	13.0

A14+3*A15+A16+A36 [377]

$C_7H_{12}O_4$ 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]

$C_7H_{14}N_2O_2$ pimelamide

446.8	44.56	0	99.73	102.3	44.6	45.7

5*A2*B2+2*A61 [357]

$C_7H_{14}O$ 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]

$C_7H_{16}N_2O$ 1-hexyl urea

383.0	22.4	0	58.49	78.2	22.4	30.0

A1+A67+5*A2*B2 [305]

$C_7H_{16}O$ 1-heptanol

239.9	18.35	0	76.5	75.1	18.4	18.0

A1+6*A2*B2+A30 [293]

$C_7H_{16}O$ propyl *tert*-butyl ether

179.6	9.87	0	55.0	59.2	9.9	10.6

4*A1+A2+A4*B4+A32 [20, 308]

$C_7H_{16}O$ isopropyl *tert*-butyl ether

184.8	8.46	0	45.78	59.9	8.46	11.1

5*A1+A4*B4+A32+A3*B3 [20, 308]

$C_7H_{18}N_2$ heptane-1,7-diamine

298.5	36.95	0	123.8	107.9	37.0	32.2

7*A2*B2+2*A45 [15]

$C_8Cl_4N_2$ 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]

$C_8H_5NO_2$ 1*H*-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]

$C_8H_5NO_2$ 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]

$C_8H_5NO_3$ 2*H*-1,3-benzoxazine-2,4(3*H*)-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_8H_6ClN 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]

$C_8H_6ClNS_2$ 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]

$C_8H_6Cl_2O_3$ 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]

$C_8H_6F_{12}O_4$ 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]

$C_8H_6O_3$ 4-formylbenzoic acid

452.2	21.3	0	47.10	52.3	21.3	23.7

4*A10+2*A12+A36*B36+A34 [230]

$C_8H_6S_2$ 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]

$C_8H_6O_4$ 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]

$C_8H_7ClN_2O_2$ 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]

$C_8H_7ClO_2$ 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]

$C_8H_7ClO_2$ 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]

$C_8H_7ClO_2$ 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_8H_8BrNO 4-bromoacetanilide

441.2	25.8	0	58.48	51.2	25.8	22.6

4*A10+2*A12+A1+A60+A21 [243]

$C_8H_8N_2$ 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]

$C_8H_8N_2O_2$ 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]

$C_8H_8O_2$ phenylacetic acid

349.2	15.2	0	43.5	47.9	15.2	16.7
5*A10+A11+A2+A36						[2]

$C_8H_8O_2$ 4’-hydroxyacetophenone

382.8	18.08	0	47.2	57.1	18.1	21.9
4*A10+2*A12+A31+A35+A1						[448]

$C_8H_8O_3$ 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]

$C_8H_8O_3$ 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]

$C_8H_8O_3$ 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]

$C_8H_8O_3$ methyl 4-hydroxybenzoate

399.2	25.3	0	63.4	60.2	25.3	24.0
4*A10+2*A12+A1+A31+A38						[438]

$C_8H_8O_3$ 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_8H_8S 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]

$C_8H_9ClN_2O$ 2-chloro-N,N-dimethylnicotinamide

342.2	21.39	0	62.51	76.4	21.39	26.1

	3*A10+2*A12+2*A1+A41+A62+A22*D22					[334]
C_8H_9NO	acetanilide					
387.2	18.3	0	47.26	48.6	18.3	18.8
	5*A10+A12+A1+A60					[243]
$C_8H_9NO_2$	4-(acetylamino)phenol (acetaminophen)					
441.9	26.49	0	59.8	54.0	26.5	23.9
	4*A10+A60+A1+2*A12+A31					[350]
$C_8H_9NO_2$	2-amino-3-methylbenzoic acid					
447.4	27.30	0	61.02	52.8	27.30	23.6
	A1+3*A10+2*A12+A11+A45+A36*B36					[8]
$C_8H_9NO_2$	2-amino-5-methylbenzoic acid					
450.0	27.63	0	61.40	52.8	27.63	23.8
	A1+3*A10+2*A12+A11+A45+A36*B36					[8]
$C_8H_9NO_2$	2-amino-6-methylbenzoic acid					
398.7	27.49	0	69.0	52.8	27.5	21.1
	A1+3*A10+2*A12+A11+A45+A36*B36					[8]
$C_8H_9NO_2$	3-amino-2-methylbenzoic acid					
458.8	38.47	0	83.9	52.8	38.5	24.2
	A1+3*A10+2*A12+A11+A45+A36*B36					[8]
$C_8H_9NO_2$	3-amino-4-methylbenzoic acid					
438.8	26.89	0	61.3	52.8	26.9	23.2
	A1+3*A10+2*A12+A11+A45+A36*B36					[8]
$C_8H_9NO_2$	4-amino-3-methylbenzoic acid					
439.4	21.77	0	49.5	52.8	21.8	23.2
	A1+3*A10+2*A12+A11+A45+A36*B36					[8]
$C_8H_9NO_2$	3-aminophenylacetic acid					
468.2	42.7	0	91.2	57.2	42.7	26.8
	4*A10+A11+A12+A45+A36*B36+A2					[2]
$C_8H_9NO_2S_2$	N-theonylthiocarbamic-O-ethyl ester					
345.9	21.90	0	63.3	54.6	21.9	18.9
	A14+2*A15+A131+2*A18+A18*B18+A19+A60+A176+A1+A2					[403]

$C_8H_9N_3O_2$	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]
$C_8H_{10}Cl_2O_2$	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]
$C_8H_{10}N_2O_3$	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]
$C_8H_{10}N_2O_3S$	sulfacetamide					
455.2	29.8	0	65.5	65.5	29.8	29.8
4*A10+2*A12+A1+A45+A173						[168]
$C_8H_{10}N_2O_4S$	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]
$C_8H_{10}N_2O_4S$	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]
$C_8H_{10}N_4O_2$	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]
$C_8H_{10}O$	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]
$C_8H_{10}O_3$	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]
$C_8H_{11}N_3O_4$	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]
$C_8H_{12}N_2$	suberonitrile					
268.9	21.97	0	81.70	91.2	21.97	24.5
	6*A2*B2+2*A56					[402]
$C_8H_{12}OS$	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]
$C_8H_{12}O_2$	2,6-dioxaadamantane					
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]
$C_8H_{12}S_6$	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]
$C_8H_{14}O_2$	cyclohexylacetic acid					
302.6	13.80	0	45.60	43.2	13.80	13.1
	A14+3*A15+A36+A16					[377]
$C_8H_{14}O_4$	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]
$C_8H_{15}N_5S$	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]
$C_8H_{15}N_7O_2S_2$	N'(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	
	prediction not made						[23]
C_8H_{16}		ethylcyclohexane					
	161.5	8.5	0	52.6	54.5	8.5	8.80
	A14+A16+A1+A2+3*A15						[368]
$C_8H_{16}N_2O_2$		suberamide					
	431.3	5.45	12.64				
	493.2	58.4	118.4	131.0	111.6	63.9	55.0
	6*A2*B2+2*A61						[357]
$C_8H_{16}O$		cyclooctanol					
	264.1	2.05	7.76				
	297.1	1.97	6.63	14.39	38.9	4.02	11.6
	A14+5*A15+A16+A30						[220]
$C_8H_{16}S_4$		1,4,7,10-tetrathiacyclododecanone					
	499.2	31.0	0	62.10	67.2	31.0	33.5
	A14+6*A15+4*A131						[1]
$C_8H_{17}NO$		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
	A1+6*A2*B2+A61						[391]
$C_8H_{18}N_2O$		1-heptyl urea					
	386.1	29.0	0	75.1	87.5	29.0	33.8
	A1+A67+6*A2*B2						[305]
$C_8H_{18}O$		1-octanol					
	258.4	25.24	0	97.7	84.4	25.2	21.8
	A1+7*A2*B2+A30						[293]
$C_8H_{18}O$		isobutyl *tert*-butyl ether					
	162.3	8.65	0	53.3	48.6	8.7	7.9
	5*A1+A32+A4+A3+A2						[332]
$C_8H_{18}O_2$		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]

$C_8H_{19}NSi$ triethylsilylethyleneimine

183.6 14.25 0 77.6 61.1 14.3 11.2

+A14+A119+A109+3*A1+3*A2 [21]

$C_8H_{20}N_2$ octane-1,8-diamine

324.8 50.98 0 157.0 117.2 51.0 38.1

8*A2*B2+2*A45 [15]

$C_9H_6N_2O_3$ 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]

$C_9H_6O_2$ 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]

$C_9H_7BrO_2$ 3-bromo-*trans*-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_9H_7NO 8-quinolinol

346.8 22.1 0 63.7 53.1 22.1 18.4

6*A10+3*A12+A41+A31 [33]

$C_9H_7NO_2$ 1-methyl-1*H*-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]

$C_9H_8Cl_2O_3$ 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]

$C_9H_8Cl_2O_3$ 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_9H_8O 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_9H_8O	2-indanone					
330.0	16.89	0	50.7	48.1	16.9	15.9
4*A10+A14+3*A15+2*A19+A114						[388]
$C_9H_8O_2$	*trans*-cinnamic acid					
406.1	22.21	0	54.7	52.2	22.2	21.2
5*A10+A12+A6+A36+A6*B6						[416]
$C_9H_8O_3$	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]
$C_9H_8O_4$	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]
$C_9H_8O_4$	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]
$C_9H_8O_4$	monomethyl phthalate					
357.5	21.63	0	60.5	56.1	21.6	20.1
4*A10+2*A12+A1+A38+A36*B36						[330]
$C_9H_8O_4$	monomethyl isophthalate					
466.7	36.50	0	78.2	56.1	36.5	26.2
4*A10+2*A12+A1+A38+A36*B36						[330]
$C_9H_8O_4$	monomethyl terephthalate					
492.5	37.68	0	76.5	56.1	37.7	27.6
4*A10+2*A12+A1+A38+A36*B36						[330]
$C_9H_9N_3O_2S_2$	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]
$C_9H_{10}N_2$	N-(2-cyanoethyl)aniline					
310.6	0.98	3.16				

323.3	19.4	60.01	63.17	65.8	20.38	21.3
4*A10+A11+A12+2*A2+A45+A56						[287]

$C_9H_{10}N_2O_3$ 2-(hydroxyimino)-N-(4-methoxyphenyl)acetamide

457.6	8.3	0	18.14	56.0	8.3	25.6
4*A10+2*A12+A1+A32+A60+A6*B6+A53						[102]

$C_9H_{10}N_2O_3$ 2-(hydroxyimino)-N-(2-methoxyphenyl)acetamide

424.6	27.8	0	65.47	56.0	27.8	23.8
4*A10+2*A12+A1+A32+A60+A6*B6+A53						[102]

$C_9H_{10}N_2O_3$ 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
2*A1+3*A10+2*A12+A11+A50+A60						[24]

$C_9H_{10}O_3$ 4-hydroxy-3-ethoxybenzaldehyde (ethyl vanillin)

349.8	23.1	0	66.0	70.9	23.1	24.8
3*A10+3*A12+A31+A34+A1+A32+A2						[440]

$C_9H_{10}O_3$ 4-methyl-4-cyclohexene-1,2-dicarboxylic anhydride

335.5	17.67	0	52.7	54.5	17.7	18.3
2*A14+3*A15+A1+A18+A19+2*A16+A117						[302]

$C_9H_{10}O_3$ 3,4-dimethoxybenzaldehyde

317.0	20.3	0	64.1	65.8	20.3	20.9
3*A10+3*A12+2*A1+2*A32+A34						[440]

$C_9H_{10}O_3$ 1,4-benzodioxan-2-hydroxymethyl

362.4	28.78	0	79.4	64.2	28.8	23.3
A14+3*A15+2*A19+4*A10+A16+A2+A30*D30						[414]

$C_9H_{10}O_3$ ethyl 4-hydroxybenzoate

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
4*A10+2*A12+A1+A31+A38*B38+A2						[437, 438]

$C_9H_{11}ClN_2O$	N,N-dimethyl-N'-(4-chlorophenyl)urea (Monuron)					
447.6	29.3	0	65.5	66.0	29.3	29.5
2*A1+A64 +A22*D22+2*A12+4*A10						[210]
$C_9H_{11}NO$	2-(acetylamino)toluene					
382.7	21.70	0	56.70	49.2	21.70	18.8
2*A1+4*A10+A11+A12+A60						[306, 307]
$C_9H_{11}NO$	4-(acetylamino)toluene					
424.0	28.93	0	68.23	49.2	28.93	20.9
2*A1+4*A10+A11+A12+A60						[306, 307]
$C_9H_{11}NO_2S_2$	N-theonylthiocarbamic-O-propyl ester					
370.1	26.10	0	70.52	61.7	26.1	22.8
A14+2*A15+A131+2*A18+A18*B18+A19+A176+A1+2*A2						[403]
$C_9H_{12}N_2S$	2-propyl-4-pyridinecarbothioamide					
414.1	23.21	0	56.05	62.8	23.2	26.0
3*A10+A11+A12+A41+A92+A1+2*A2						[444]
C_9H_{12}	trispiro[2.0.2.0.2.0]nonane ([3] rotane)					
312.1	14.14	0	45.3	18.7	14.1	5.8
4*A14-3*A15+3*A17						[190]
$C_9H_{12}O_4$	3,4,5-trimethoxyphenol					
420.2	31.94	0	76.0	72.0	31.9	30.3
3*A1+A31+3*A32+2*A10+4*A12						[410]
$C_9H_{14}N_2$	azelanitrile					
251.1	18.68	0	74.4	100.5	18.7	25.2
7*A2*B2+2*A56						[402]
$C_9H_{14}O$	2-oxaadamantane					
567.0	8.12	0	14.3	46.3	8.1	26.3
3*A14+A15+4*A16+A112						[26]
$C_9H_{14}S$	2-thiaadamantane					
211.0	1.95	9.24				
597.0	8.10	14.0	22.81	48.0	10.1	27.8
3*A14+A15+4*A16+A131						[26]

$C_9H_{16}O_4$	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]
$C_9H_{17}N_5S$	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_9H_{18}	propylcyclohexane					
178.0	10.6	0	59.6	61.6	10.6	11.0
	A14+A16+A1+2*A2+3*A15					[368]
$C_9H_{18}N_2O_2$	azelamide					
450.4	55.0	0	122.11	120.9	55.0	54.5
	7*A2*B2+2*A61					[357]
$C_9H_{18}S_4$	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]
$C_9H_{20}N_2O$	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]
$C_9H_{20}O_2$	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]
$C_9H_{20}O_2S_2$	*meso* 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]
$C_9H_{20}O_2S_2$	racemic 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]

$C_9H_{21}As$	tripropylarsine					
180.0	14.60	0	81.11	95.8	14.60	17.7
3*A1+6*A2+A98						[13]
$C_9H_{22}N_2$	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]
$C_{10}H_2Cl_6$	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]
$C_{10}H_3Cl_5$	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]
$C_{10}H_3Cl_5$	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]
$C_{10}H_3Cl_5$	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]
$C_{10}H_3Cl_5$	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]
$C_{10}H_3Cl_5$	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]

$C_{10}H_3Cl_5$	1,2,4,6,7-pentachloronaphthalene					
404.3	22.58	0	55.9	50.7	22.6	20.5
3*A10+7*A12+5*A22*D22						[356]
$C_{10}H_3Cl_5$	1,2,4,6,8-pentachloronaphthalene					
429.0	19.75	0	46.0	50.7	19.8	21.8
3*A10+7*A12+5*A22*D22						[356]
$C_{10}H_4Cl_4$	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
4*A10+6*A12+4*A22*D22						[356]
$C_{10}H_4Cl_4$	1,2,7,8-tetrachloronaphthalene					
401.3	14.62	0	36.43	49.4	14.6	19.8
4*A10+6*A12+4*A22*D22						[356]
$C_{10}H_4Cl_4$	1,3,5,7-tetrachloronaphthalene					
453.0	27.14	0	59.91	49.4	27.1	22.4
4*A10+6*A12+4*A22*D22						[356]
$C_{10}H_5Cl_3$	1,2,3-trichloronaphthalene					
354.7	18.44	0	51.99	48.1	18.4	17.1
5*A10+5*A12+3*A22*D22						[356]
$C_{10}H_6F_3NO_2$	4-trifluoromethyl-7-aminocoumarin					
494.8	31.7	0	64.1	62.1	31.7	30.7
A14+3*A15+3*A10+A12+A45+A115+A18+3*A19+3*A25+A4*B4						[118]
$C_{10}H_8$	naphthalene					
353.4	16.44	0	46.5	44.2	16.4	15.6
8*A10+2*A12						[439]
$C_{10}H_9N$	2-methylquinoline					
270.5	12.52	0	46.3	48.3	12.5	13.1
A1+6*A10+2*A12+A11+A41						[291]
$C_{10}H_9N$	8-methylquinoline					
246.9	10.73	0	43.46	48.3	10.7	11.9
A1+6*A10+2*A12+A11+A41						[291]

$C_{10}H_{10}$ 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

5*A14-4*A15+8*A16+2*A18 [171]

$C_{10}H_{10}$ 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

3*A14+A15+4*A16+6*A18 [171]

$C_{10}H_{10}$ 2,2a,2b,3,5a,5b-hexahydro-1,2,3-metheno-1*H*-cycloprop[cd]indene (snoutene)

334.0	7.87	0	23.56	74.0	7.87	24.7

4*A14-2*A15+6*A16+2*18 [171]

$C_{10}H_{10}$ 1,2-dihydronaphthalene

264.4	10.53	0	39.8	46.3	10.5	12.2

A14+3*A15+2*A18+2*A19+4*A10 [409]

$C_{10}H_{10}Cl_2O_3$ 4-(2,4-dichlorophenoxy)butanoic acid

395.5	35.0	0	88.50	86.2	35.0	34.1

3*A10+2*A12+A11+3*A2+2*A22*D22+A36*D36+A32 [289]

$C_{10}H_{10}N_2$ 1,8-diaminonaphthalene

339.8	16.15	0	47.5	57.2	16.2	19.4

6*A10+4*A12+2*A45 [398]

$C_{10}H_{10}N_4O_2S$ sulfadiazine

532.7	44.3	0	83.2	79.1	44.3	42.1

7*A10+3*A12+2*A41+A95+A45 [168]

$C_{10}H_{10}O_2$ *trans* methyl cinnamate

309.0	33.1	0	107.1	64.1	33.1	19.8

A1+5*A10+A12+A38+A6+A6*B6 [39]

$C_{10}H_{10}O_2$ 4-methoxycinnamaldehyde

332.7	19.0	0	57.2	69.0	19.0	23.0

4*A10+2*A12+A1+A32+A34+2*A6 [440]

$C_{10}H_{10}O_3$ 2-methoxycinnamic acid

458.7	32.54	0	70.9	62.4	32.5	28.6

4*A10+2*A12+A6+A36*B36+A6*B6+A1+A32 [111]

$C_{10}H_{10}O_3$	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]
$C_{10}H_{11}N_3O_3S$	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						

$C_{10}H_{12}N_2O_3$	N-(4-ethoxyphenyl)-2-(hydroxyimino)acetamide					
491.2	7.6	0	15.5	63.1	7.6	31.0
4*A10+2*A12+A1+A32+A60+A6*B6+A53+A2						[102]
$C_{10}H_{12}N_2O_3$	N-(2-ethoxyphenyl)-2-(hydroxyimino)acetamide					
424.6	27.8	0	65.5	63.1	27.8	26.8
4*A10+2*A12+A1+A32+A60+A6*B6+A53+A2						[102]
$C_{10}H_{12}N_2O_4$	(2-hydroxyethyl)[3-[(hydroxyimino)methyl]phenyl carbamic acid					
508.3	28.9	0	56.9	56.9	28.9	28.9
3*A10+2*A12+A11+2*A2+A6*B6+A53+A30*C30+A178						[102]
$C_{10}H_{12}O_2$	2,3,5,6-tetramethyl-1,4-benzoquinone					
384.1	18.39	0	47.9	62.9	18.4	24.2
4*A1+A14+3*A15+4*A19+2*A114						[202]
$C_{10}H_{12}O_2$	2-isopropyl-5-methyl-1,4-benzoquinone (thymoquinone)					
323.2	18.16	0	56.2	47.4	18.2	15.3
3*A1+A14+3*A15+2*A19+2*A18*B18+2*A114+A3						[232]
$C_{10}H_{12}O_3$	propyl 4-hydroxybenzoate					
369.3	27.2	0	73.7	74.4	27.2	27.5
4*A10+2*A12+A1+A31+A38*B38+2*A2						[438]
$C_{10}H_{12}O_5$	2,4,5-trimethoxybenzoic acid					
417.9	31.15	0	74.5	81.9	31.2	34.2
3*A1+2*A10+4*A12+3*A32+A36*D36						[306, 307]
$C_{10}H_{12}O_5$	3,4,5-trimethoxybenzoic acid					
444.5	29.90	0	67.3	81.9	29.9	36.4
3*A1+2*A10+4*A12+3*A32+A36*D36						[306, 307]
$C_{10}H_{13}NO_2$	4-ethoxyacetanilide					
410.2	21.4	0	52.2	63.1	21.4	25.9
2*A1+4*A10+2*A12+A32+A60+A2						[243]
$C_{10}H_{13}NO_2S_2$	N-theonylthiocarbamic-O-butyl ester					
364.3	23.89	0	65.6	68.8	23.9	25.1
A14+2*A15+A131+2*A18+A18*B18+A19+A60+A176+A1+3*A2						[403]
$C_{10}H_{13}N_5O_4$	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]
$C_{10}H_{14}N_4O_3$		(R,S)-3,7-dihydro-7-(2-hydroxypropyl)-1,3-dimethyl-1*H*-pyrine-2,6-dione					
		(Proxyphylline)					
(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.]					
$C_{10}H_{15}N_5O_3$		9-(4-hydroxy-3-hydroxymethylbut-1-yl)quanine (Penciclovir) [39809-25-1]					
	551.2	35.74	0	64.84		35.74	
		prediction not made					[212]
$C_{10}H_{16}$		*exo* 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]
$C_{10}H_{16}$		*endo* 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]
$C_{10}H_{16}$		*endo* 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	30.9
	8*A2*B2+2*A56					[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	14.9
	3*A14+A15+3*A16+A17+A30					[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	26.6
	3*A14+A15+4*A16+A30					[131]
$C_{10}H_{16}O_2$	chrysanthemic acid					
390.7	14.51	0	37.1	47.8	14.5	18.7
	A14+4*A1+A17+2*A16+A7+A6+A36					[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]
$C_{10}H_{17}N_5O_3$	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	12.4
	2*A14+4*A15+2*A16					[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	43.2
	Independent value from another reference					

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]
$C_{10}H_{19}N_5S$	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]
$C_{10}H_{20}N_2O_2$	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]
$C_{10}H_{20}N_2O_2$	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-1*H*-pyrine-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*A14+5*A15+A112+A119+A131+A118+3*A19+4*A10+A84						[84]
$C_{11}H_{12}N_4O_2S$		Sulfamerazine					
	508.5	41.3	0	81.2	79.7	41.3	40.5
	6*A10+3*A12+A11+A1+2*A41+A95+A45						[168]
$C_{11}H_{14}O_3$		butyl 4-hydroxybenzoate					
	341.8	26.6	0	77.8	81.5	26.6	27.9
	4*A10+2*A12+A1+A31+A38*B38+3*A2						[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*A10+2*A12+3*A2+A1+A38+A45						[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*A10+2*A12+A2+2*A1+A3+A38+A45						[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
	A14+2*A15+A131+2*A18+A18*B18+A19+A176+A1+4*A2						[403]
$C_{11}H_{15}N_3O_2$		N-caproylpyrazinamide					
	351.7	35.95	0	102.2	92.9	35.95	32.7
	3*A10+A12+2*A41+4*A2+A1+A71						[86]
$C_{11}H_{16}N_2O_2$		N-methyl-N-(4-*tert*-butylphenyl)nitramine					
	351.2	23.4	0	66.63	58.4	23.4	20.5
	4*A1+A4+4*A10+A11+A12+A47+A51						[127]
$C_{11}H_{18}N_2$		undecanedinitrile					
	266.1	26.0	0	97.71	119.1	26.0	31.7
	9*A2*B2+2*A56						[402]
$C_{11}H_{22}N_2O_2$		undecandiamide					
	451.2	64.4	0	142.7	139.5	64.4	62.9
	9*A2*B2+2*A61						[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]
$C_{11}H_{24}N_2O$	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]
$C_{12}H_8N_2$	1,10-phenanthroline					
391.1	11.8	0	30.2	51.0	11.8	19.9
	8*A10+4*A12+2*A41					[426]
$C_{12}H_8O$	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]
$C_{12}H_8OS$	phenoxathiin					
329.6	19.43	0	59.0	58.6	19.4	19.3
	3*A15+A14+4*A19+8*A10+A131+A112					[389]
$C_{12}H_8O_2S$	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]
$C_{12}H_9Cl_2NO_3S$	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]
$C_{12}H_9F_3N_2O_2$	Leflunomide					
438.2	32.43	0	74.0	63.4	32.4	27.8

	3*A25+A4*B4+4*A10+A11+A12+A60+A14+2*A15+A1+2*A19+ A18*B18+A118+A112					[354]
$C_{12}H_9NO$	2-benzoylpyridine					
316.5	20.91	0	66.1	67.1	20.91	21.2
	9*A10+2*A12+A41+A35					[361]
$C_{12}H_{10}ClNO_3S$	N-(2-chlorophenyl)benzenesulfonamide					
398.2	33.5	0	84.1	66.9	33.5	26.6
	9*A10+3*A12+A22*D22+A95					[373]
$C_{12}H_{10}ClNO_3S$	N-(4-chlorophenyl)benzenesulfonamide					
394.6	25.8	0	65.4	66.9	25.8	26.4
	9*A10+3*A12+A22*D22+A95					[373]
$C_{12}H_{10}ClN_3S$	N-2-pyridyl-N'-(2-chlorophenyl) thiourea					
429.7	28.3	0	65.9	71.6	28.3	30.8
	8*A10+3*A12+A41+A22*D22+A90					[4]
$C_{12}H_{10}ClN_3S$	N-2-pyridyl-N'-(4-chlorophenyl) thiourea					
462.2	34.3	0	74.2	71.6	34.3	33.1
	8*A10+3*A12+A41+A22*D22+A90					[5]
$C_{12}H_{10}CrO_3$	α-methylstyrenetricarbonyl chromium					
360.0	27.4	0	76.1	74.5	27.4	26.8
	5*A10+A12+A5+A7+A182+A1					[167]
$C_{12}H_{10}F_3NO_2$	4-(trifluoromethyl)-7-(N-ethylamino)coumarin					
432.5	30.47	0	70.5	58.7	30.5	25.4
	+A14+3*A15+A115+3*A19+A18*B18+3*A10+A12+A44+A1+ A2+A4*B4+3*A25					[118]
$C_{12}H_{10}F_3NO_2$	4-(trifluoromethyl)-7-(N,N-dimethylamino)coumarin					
420.5	26.25	0	62.4	52.3	26.3	22.0
	A14+3*A15+A115+3*A19+A18*B18+3*A10+A12+A43+ 2*A1+A4*B4+3*A25					[118]
$C_{12}H_{10}O_2S$	4,4'-thiodiphenol					
432.9	31.04	0	71.7	71.9	31.0	31.1
	8*A10+4*A12+2*A31+A84					[72]

$C_{12}H_{11}N_3S$		N-2-pyridyl-N'-phenylthiourea					
	????	41.0	0		58.2[a]	41.0	
	9*A10+3*A12+A41+A90						[6]
$C_{12}H_{11}O_2P$		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-(*p*-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]

$C_{12}H_{12}N_2O_3$ 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]

$C_{12}H_{12}N_2O_3$ 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]

$C_{12}H_{13}NO_2S$ 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]

$C_{12}H_{14}N_4O_2S$ 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]

$C_{12}H_{15}N_3O_6$ 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]

$C_{12}H_{16}N_2OS$ 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]

$C_{12}H_{16}N_2O_4$ 2,4-dinitro-1,3-dimethyl-5-*tert*-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]

$C_{12}H_{17}NO_2S_2$ 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]

$C_{12}H_{18}N_2O$ N'-(*p*-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]

$C_{12}H_{20}N_2O_2$ (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]
$C_{12}H_{24}N_2O_2$		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]
$C_{12}H_{26}N_2O$		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]
$C_{13}H_8Cl_2O$	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]
$C_{13}H_8Cl_2N_2O_4$	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]
$C_{13}H_8F_2O_3$	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]
$C_{13}H_9NO$	9(10*H*)-acridinone						
	640.0	32.5	0	50.8	55.3	32.5	35.4
	8*A10+A14+3*A15+4*A19+A121+A114						[180]
$C_{13}H_{10}BrN_3O_4$	2-cyano-6-nitro-1(2*H*)-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]
$C_{13}H_{10}ClN_3O_4$	2-cyano-6-nitro-1(2*H*)-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]

$C_{13}H_{10}N_2O_4$		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*H*-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*H*-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]

$C_{13}H_{11}N_3O_2S$ 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]

$C_{13}H_{11}N_3O_4$ 2-cyano-6-nitro-1(2*H*)-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]

$C_{13}H_{12}ClN_2O_2$ 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]

$C_{13}H_{12}ClN_3S$ 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]

$C_{13}H_{12}ClN_3S$ 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]

$C_{13}H_{12}ClN_3S$ 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]

$C_{13}H_{12}ClN_3S$ 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]

$C_{13}H_{12}ClN_3S$ 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]

$C_{13}H_{12}ClN_3S$ 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]

$C_{13}H_{12}ClN_3S$	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]
$C_{13}H_{12}ClN_3S$	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]
$C_{13}H_{12}N_2O_2$	N-methyl-N-(4-biphenylyl)nitramine						
	415.1	24.0	0	57.8	54.4	24.0	22.6
	9*A10+3*A12+A51+A47						[127]
$C_{13}H_{12}N_2O_2$	2-cyano-1(2*H*)-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]
$C_{13}H_{13}N_3O$	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.]						
$C_{13}H_{13}N_3S$	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]

$C_{13}H_{15}Cl_2N_3$ 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-2*H*-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]

$C_{13}H_{18}Br_2N_2O$ *trans*-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]
$C_{13}H_{28}N_2O$	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]
$C_{14}H_{10}N_2O_3$	10-methyl-2-nitroacridin-9(10*H*)-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]
$C_{14}H_{11}BrN_2S$	N-(4-bromophenyl)-4*H*-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]
$C_{14}H_{11}ClN_2S$	N-(4-chlorophenyl)-4*H*-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*H*)-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]

$C_{14}H_{11}N_3O_4$ 2-cyano-6-nitro-1(2*H*)-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]

$C_{14}H_{11}N_3O_4$ 2-cyano-6-nitro-1(2*H*)-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]

$C_{14}H_{12}N_2O_4$ 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*H*-furo[3,2g][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]

$C_{14}H_{13}N_3O_4$ 2-cyano-6-nitro-1(2*H*)-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]

$C_{14}H_{13}N_3O_4$ 2-cyano-6-nitro-1(2*H*)-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]

$C_{14}H_{14}ClN_2O_2$ 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]

$C_{14}H_{14}ClN_3S$ 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]

$C_{14}H_{14}ClN_3S$ 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]

$C_{14}H_{14}F_3NO_2$ 4-trifluoromethyl-7-(N,N-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]

$C_{14}H_{14}N_2O_2$ 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]

$C_{14}H_{14}N_2O_3$ 2-cyano-6-methoxy-1(2*H*)-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*H*-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*H*-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]
$C_{14}H_{15}N_3S$		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]
$C_{14}H_{15}N_3S$		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]
$C_{14}H_{15}N_3S$		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]
$C_{14}H_{15}N_3S$		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]
$C_{14}H_{16}ClN_3O$		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]
$C_{14}H_{17}N_5O_3$		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]

$C_{14}H_{18}N_2O_5$	3,5-dinitro-2,6-dimethyl-4-*tert*-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]
$C_{14}H_{19}N_2O_2$	(1RS, 2RS)-1-(4-chlorophenoxy)-3,3-dimethyl-1-(1*H*-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]
$C_{14}H_{19}N_2O_2$	(1RS,2SR)-1-(4-chlorophenoxy)-3,3-dimethyl-1-(1*H*-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]
$C_{14}H_{20}N_2O_2$	1-(1*H*-indol-4-yloxyl)-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-*tert*-butyl-o-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]
$C_{14}H_{22}N_2O_3$	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]
$C_{14}H_{22}N_4O_6$	N,N'-*bis*(2-oxo-3-oxazolidin-3-ylcarbonyl)-1,6-hexanediamine (N,N'-1,6-hexanediylbis[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]

$C_{14}H_{28}N_2O_2$ N,N,N',N'-tetrapropyloxamide

317.2	21.0	0	66.2	104.8	21.0	33.2
4*A1+8*A2+ 2*A59						[27]

$C_{14}H_{28}N_2O_2$ 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]

$C_{14}H_{30}N_2O$ 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-4*H*-1-benzoyran-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-4*H*-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]

$C_{15}H_{11}Cl_2N_2O_2$ 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]

$C_{15}H_{12}ClN_2O_2$ 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]

$C_{15}H_{12}N_2O_2$ 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]

$C_{15}H_{13}ClN_2S$` N-(2-methyl-4-chlorophenyl)-4*H*-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(10*H*)-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(10*H*)-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-1*H*-pyrrolizine-1-carboxylic acid (Ketoroloc)

(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

crystalline forms

(III) 426.2 25.42 0 59.6 84.1 25.4 35.8
2*A14+4*A15+2*A19+2*A18+A119+A16+A36*D36+A35+5*A10+A12 [263]

$C_{15}H_{14}N_2OS$ N-(4-methoxyphenyl)-4*H*-3,1-benzothiazin-2-amine
436.2 16.1 0 36.9 72.2 16.1 31.5
A14+3*A15+3*A19+A131+A118+8*A10+2*A12+A44+A1+A32 [228]

$C_{15}H_{14}N_2S$ N-(4-methylphenyl)-4*H*-3,1-benzothiazin-2-amine
448.4 19.9 0 44.4 65.4 19.9 29.3
A14+3*A15+3*A19+A131+A118+8*A10+A11+A12+A44+A1 [228]

$C_{15}H_{14}O_3$ 4-(phenylmethoxy)benzeneacetic acid
396.1 29.3 0 74.0 75.0 29.3 29.7
9*A10+2*A11+A12+2*A2+A32+A36*B36 [422]

$C_{15}H_{14}O$ 5*H*-10,11-dihydrodibenzo[a,d]cyclohexane-5-ol
365.2 19.0 0 52.0 45.2 19.0 16.5
A14+4*A15+8*A10+4*A19+A16+A30 [333]

$C_{15}H_{15}ClO_5$ 8-(hydroxymethyl)-6-chloro-5,7-dimethyl-2-oxo-2*H*-1-benzopyran-3-carboxylic acid, ethyl ester
446.5 3.59 8.0
456.4 25.08 55.0 62.99 86 28.7 39.2
A14+3*A15+3*A19+A18+A115+3*A11+A12+2*A2+3*A1+A30*D30+
A22*D22+A38 [129]

$C_{15}H_{15}N_3O_3$ 6-(acetylamino)-2-cyano-1(2*H*)-quinolinecarboxylic acid, ethyl ester
441.2 35.02 0 79.4 56.0 35.0 24.7
A14+3*A15+3*A10+A12+2*A19+2*A18+A16+A60+A56+A2+2*A1+A169 [274]

$C_{15}H_{15}N_3O_4$ 2-cyano-6-nitro-1(2*H*)-quinolinecarboxylic acid, butyl ester
359.1 25.16 0 70.1 68.8 25.2 24.7
A14+3*A15+3*A10+A12+2*A19+2*A18+A16+A50+3*A2+A1+A56+A169 [274]

$C_{15}H_{15}N_3O_4$ 2-cyano-6-nitro-1(2*H*)-quinolinecarboxylic acid, 2-methylpropyl ester
388.8 28.26 0 72.7 62.4 28.3 24.2
A14+3*A15+3*A10+A12+2*A19+2*A18+A16+A50+A56+A2+2*A1+
A3*B3+A169 [274]

$C_{15}H_{16}ClN_2O_2$ 4-chloro-2'-hydroxy-4'-propoxyazobenzene

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]

$C_{15}H_{16}N_2O_2$ 2-cyano-1(2*H*)-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]

$C_{15}H_{16}N_2O_2S$ 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]

$C_{15}H_{16}N_2O_3$ 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]

$C_{15}H_{16}N_2O_3$ 2-cyano-6-methoxy-1(2*H*)-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]

$C_{15}H_{16}N_4O_6$ 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*H*-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]

$C_{15}H_{20}N_4O_4$ 1,1'-(1,5-pentanediyl)-*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-*tert*-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*H*-pyrano[4,3-j]-1,2-benzodioxepin-10(3*H*)-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	50.1

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	28.27

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	41.5

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	59.1

A1+A67+13*A2*B2 [305]

$C_{15}H_{32}O$ 1-pentadecanol

316.4	29.6	0	93.6	149.5	29.6	47.3

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	32.8

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	27.1

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	17.4

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*H*-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]
$C_{16}H_{13}ClN_2O$		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]
$C_{16}H_{14}N_2OS$		N-(4-acetylphenyl)-4*H*-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]
$C_{16}H_{14}N_2O_3S$		4-(5-methyl-3-phenyl-4-isoxazolyl)benzenesulfonamide (Valdecoxib)					
	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-dihyro-5,7-dihyroxy-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]

$C_{16}H_{16}N_2O_2$ 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]

$C_{16}H_{16}N_2O_4$ 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-7*H*-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-7*H*-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]

$C_{16}H_{16}O_2$ *trans*-9,10-*bis*hydroxymethyl-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]

$C_{16}H_{16}O_2$ *trans*-5-hydroxymethyl-5,6-dihydro-7*H*-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]

$C_{16}H_{17}N_3O_3$ 6-(acetylamino)-2-cyano-1(2*H*)-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]

$C_{16}H_{18}N_2OS$ 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]

$C_{16}H_{18}N_2O_3$ 2-cyano-6-methoxy-1(2*H*)-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]

$C_{16}H_{20}N_4O_3S$ 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-(*trans*-4-propycyclohexyl)benzonitrile

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]

$C_{16}H_{22}N_4O_4$ 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]

$C_{16}H_{24}N_2OS$ 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]

$C_{16}H_{24}N_2S_2$ 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]

$C_{16}H_{36}O_3Si_2$ 11-(1,1,3,3-tetramethyldisiloxanyl)undecanoic acid, methyl ester

233.3 23.5 0 100.7 23.5

prediction not made [343]

$C_{17}H_{10}ClN_3O_3$ 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]

$C_{17}H_{11}ClN_2O_2$ 2-cyano-1(2*H*)-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]

$C_{17}H_{12}N_2O_2$ 2-cyano-1(2*H*)-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]

$C_{17}H_{14}F_3N_3O_2S$ 4-[5-(3-methylphenyl)-3-(trifluoromethyl)-1*H*-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]

$C_{17}H_{14}O_4S$ 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]

$C_{17}H_{16}N_2O_4$ 5-phenoyxmethyl-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]

$C_{17}H_{18}ClNO_2S$ 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]

$C_{17}H_{18}N_2O_3S$ 4-methoxy-N-[[[(3-methoxyphenyl)methyl]amino]thioxomethyl]benzamide

389.2	31.02	0	79.7	79.7	31.0	31.0
8*A10+A11+3*A12+2*A1+A2+A32+A60+A174						[262]

$C_{17}H_{19}NO_4$ Fenoxycarb

326.3	26.98	0	82.68	100.2	26.98	32.7
9*A10+3*A12+2*A32+3*A2+A1+A69						[316]

$C_{17}H_{19}N_3O_3$ 6-(acetylamino)-2-cyano-1(2*H*)-quinolinecarboxylic acid, 2-methylpropyl ester

404.6	19.83	0	49.0	57.2	19.8	23.1
A14+3*A15+3*A10+A12+2*A19+2*A18+A16+A60+A56+A2+						
3*A1+A3+A169						[274]

$C_{17}H_{19}N_3O_3$ 6-(acetylamino)-2-cyano-1(2*H*)-quinolinecarboxylic acid, butyl ester

436.1	36.44	0	83.6	70.2	36.4	30.6
A14+3*A15+3*A10+A12+2*A19+2*A18+A16+A60+A56+3*A2+						
2*A1+A169						[274]

$C_{17}H_{20}N_2O_2S$ N,N'-*bis*[(3-methoxyphenyl)methyl]thiourea

354.7	33.22	0	93.7	91.6	33.2	32.5
8*A10+2*A12+2*A11+2*A2+2*A1+2*A32+A90						[262]

$C_{17}H_{22}FeO_2S_2$ 1,9-dioxa-4,6-dithiacyclundecan-5-ylferrocene

371.7	29.4	0	79.1	93.2	29.4	34.6
3*A14+12*A15+9*A18*B18+A19+A179+2*A112+2*A131+A16						[130]

$C_{17}H_{26}O_3$ 3-decyloxybenzoic acid

345.1	33.88	0	98.2	136.8	33.9	47.2
4*A10+2*A12+A32+A1+9*A2*B2+A36*B36						[126]

$C_{17}H_{28}N_2OS$ N-[(3-methoxyphenyl)methyl]-N'-octylthiourea

350.7	37.94	0	108.2	117.0	37.9	41.0
4*A10+A11+A12+A32+2*A1+8*A2+A90						[262]

$C_{17}H_{34}O_2$ 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
2*A1+14*A2*B2+A38						[193, 245]

$C_{17}H_{36}O$ 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]
$C_{18}H_{13}ClN_2O_3$		2-cyano-6-methoxy-1(2*H*)-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]
$C_{18}H_{14}F_4N_2O_4S$		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]**					

$C_{18}H_{14}N_2O_2$	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]
$C_{18}H_{14}N_2O_3$	2-cyano-6-methoxy-1(2*H*)-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-b]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]
$C_{18}H_{15}ClN_2O_2S$	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]
$C_{18}H_{18}F_3N_3O_3$	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]
$C_{18}H_{19}Cl_2NO_4$	(±) 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]

$C_{18}H_{19}Cl_2NO_4$ (+) 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]

$C_{18}H_{20}N_2O_4$ 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]

$C_{18}H_{20}N_2O_2$ 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]

$C_{18}H_{20}N_2O_4$ 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
		10*A10+2*A11+2*A1+A44+3*A3*B3+A180+A30*C30					[36]
$C_{18}H_{22}FNO_4$		(1R,2S)-ephedrinium (S)-4'-fluoromandelate					
	380.4	24.5	0	64.4	73.8	24.5	28.1
		10*A10+2*A11+2*A1+A44+3*A3*B3+A180+A30*C30					[36]
$C_{18}H_{28}S_8$		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
		2*A14+4*A15+6*A19+4*A131+4*A84+4*A1+8*A2					[49]
$C_{18}H_{30}$		1,2,4,5-tetraisopropylbenzene					
	393.0	19.60	0	49.9	60.0	19.6	23.6
		8*A1+2*A10+4*A12+4*A3					[45]
$C_{18}H_{36}O_2$		stearic acid					
	340.2	50.93	0	149.7	162.2	50.9	55.2
		16*A2*B2+A36					[135]
$C_{18}H_{36}O_2$		methyl heptadecanoate					
	304.2	48.1	0	158.1	182.4	48.1	55.5
		2*A1+15*A2*B2+A38					[245]
$C_{18}H_{37}NO$		octadecanamide					
	298.7	2.2	7.36				
	379.7	54.8	144.32	151.7	194.3	57.0	73.7
		A1+16*A2*B2+A61					[391]
$C_{18}H_{38}O$		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
		A1+17*A2*B2+A30					[208, 299]
$C_{19}H_{13}NO$		10-phenylacridin-9(10*H*)-one					
	550.0	38.9	0	70.7	63.3	38.9	34.8
		13*A10+A12+A14+3*A15+4*A19+A114+A119					[180]
$C_{19}H_{16}ClNO$		1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-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]

$C_{19}H_{16}F_8O_2$ 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-2*H*-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]

$C_{19}H_{17}ClN_2O$ 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]

$C_{19}H_{18}N_2O_3$ 1',3'-dihydro-1',3',3'-trimethyl-6-nitrospiro[2*H*-1-benzopyran-2,2'-(2*H*)-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]

$C_{19}H_{19}NO_4S$ ethyl 5-phenylsulfonyl-4,7-dihydro-4,7-ethano-2*H*-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-b]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]

$C_{19}H_{22}F_8O_2$ 2,3-*bis*(trifluoromethyl)-4-methoxyphenyl-*trans*-4-n-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-xylylformimodyl)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]

$C_{19}H_{26}FeO_2S_3$ 1,9-dioxa-4,6,12-trithiacycltetradecan-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]

$C_{19}H_{26}FeO_3S_2$ 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]

$C_{19}H_{27}NO_4$ (3R)-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]

$C_{20}H_4Cl_4F_{13}NO_2$ 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]

$C_{20}H_6Cl_2F_{13}NO_2$ 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]

$C_{20}H_6Cl_2F_{13}NO_2$ 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]

$C_{20}H_{23}N_3O_9$ N-[N-[[2-(1,3-dihydro-1,3-dioxo-2*H*-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-*tert*-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]

$C_{20}H_{27}N_5O_2$ 6-[4-(1-cyclohexyl-1*H*-tetrazol-5-yl)butoxy]-3,4-dihydro-2(1*H*)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]

$C_{20}H_{30}N_4O_4$ 1,1'-(1,10-decanediyl)*bis*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]

$C_{21}H_{20}Br_8O_2$ 2,2-*bis*[3,5-dibromo-4-(2,3-dibromopropyloxy)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-oxypropoxy)-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]
$C_{21}H_{35}N_3O_2$		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]
$C_{21}H_{36}N_2OS$		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
2*A1+A38+18*A2*B2						[245]

$C_{22}H_{16}$ 2-(biphen-4-yl)naphthalene

489.5	25.10	0	51.3	73.4	25.1	35.9
16*A10+6*A12						[406]

$C_{22}H_{16}$ 2-(biphen-3-yl)naphthalene

346.3	18.50	0	53.4	73.4	18.5	25.4
16*A10+6*A12						[406]

$C_{22}H_{19}Br_2NO_3$ Deltamethrin

372.2	26.73	0	71.8	96.5	26.7	35.9
A14+A17+2*A16+2*A1+A6+A7+2*A21+A38+A3*B3+A56+2*A12+A11+ 9*A10+A32						[316]

$C_{22}H_{21}Cl_3N_4O$ Rimonabant

427.9	36.1	0	84.4	92.3	36.1	39.5
2*A14+5*A15+A118+2*A119+3*A19+A60+5*A12+7*A10+A1+3*A22*D22						[418]

$C_{22}H_{23}NO_3$ Fenpropathrin

322.5	18.57	0	57.6	82.2	18.6	26.5
A14+A38+A3*B3+9*A10+A11+2*A12+A32+4*A1+2*A17+A16+A56						[35]

$C_{22}H_{25}NO_3$ 2-(4-nitrophenyl)-1-[4-(*trans*-4-ethylcyclohexyl)phenyl]ethanone

445.1	37.32	0	83.9	94.2	37.3	41.9
A14+3*A15+2*A16+2*A11+2*A12+8*A10+2*A2+A1+A35+A50						[153]

$C_{22}H_{25}NO_6$ methyl Naltrexone-3-O-carbonate

393.7	10.92	0	27.7	51.9	10.9	20.4
5*A14+2*A15+3*A16+2*A17+A114+A112+A119+2*A10+A12+A30*D30+A2+ 3*A19+A149+A1						[235]

$C_{22}H_{27}NO_2$ Danazol

501.8	35.5	0	70.8	62.6	35.5	31.4
5*A14+5*A15+A18+A18*B18+3*A19+A118+A112+3*A17+3*A16+A30*C30+ A8+A9+2*A1						[418]

$C_{22}H_{28}N_2O$ 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]

$C_{22}H_{33}N_3O_2$ 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]

$C_{22}H_{34}N_4O_4$ 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-dioxa-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-(*trans*-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]

$C_{23}H_{28}ClN_3O_5S$ 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-dicaproxypropyl-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-dicaproxypropyl-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]

$C_{24}H_{26}N_2O_4$ 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]

$C_{24}H_{27}NO_5S$ Troglitazone

412.4 48.8 0 118.3 118.1 48.8 48.7

2*A14+5*A15+A112+2*A19+A17+A124+A16+4*A11+2*A12+4*A10+2*A2+
A32+4*A1+A31+A167 [418]

$C_{24}H_{28}FN_3O$ N-methyl-[1-[1-(2-fluorophenethyl)piperidin-4-yl]-1*H*-indol-6-yl]acetamide

(I)	421.3	38.2	0	90.67	84.8	38.2	35.7
(II)	413.0	35.2	0	85.23	84.8	35.2	35.0

2*A14+5*A15+2*A19+A18+A18*B18+7*A10+2*A11+A12+2*A119+A16+3*A2+
A1+A24+A60 [78]

$C_{24}H_{29}NO_3$ 2-(4-nitrophenyl)-1-[4-(*trans*-4-butylcyclohexyl)phenyl]ethanone

426.9	36.40	0	85.27	115.5	36.40	49.3

A14+3*A15+2*A16+8*A10+2*A11+2*A12+A35+A50+5*A2+A1 [153]

$C_{24}H_{29}NO_6$ propyl Naltrexone-3-O-carbonate

379.2	20.97	0	55.3	66.1	21.0	25.1

5*A14+2*A15+3*A16+2*A17+A114+A112+A119+2*A10+A12+A30*D30+
3*A19+A149+A1+3*A2 [235]

$C_{24}H_{29}NO_6$ isopropyl Naltrexone-3-O-carbonate

427.2	26.62	0	62.3	59.6	26.6	25.5

5*A14+2*A15+3*A16+2*A17+A114+A112+A119+2*A10+A12+A30*D30+A2
3*A19+A149+3*A1+A3*B3 [235]

$C_{24}H_{32}O_3$ 3-[(1-oxohexyl)oxy]-estra-1,3,5(10)-trien-17-one

370.0	23.0	0	62.16	96.3	23.0	35.6

3*A14+34*A15+2*A19+3*A16+A17+3*A10+A12+A114+A38+2*A1+4*A2 [116]

$C_{24}H_{32}O_8$ dibenzo-24-crown-8

375.5	62.5	0	166.4	130.7	62.5	49.1

8*A10+A14+21*A15+8*A112+4*A19 [133, 295]

$C_{24}H_{34}N_4O_5S$ Glimepiride

485.7	53.3	0	109.7	105.8	53.3	51.4

2*A14+5*A15+2*A19+2*A16+A125+2*A60+A95+3*A1+3*A2+4*A10+
A11+A12 [418]

$C_{24}H_{36}O_5$ Lovastatin

444.3	36.53	0	82.2	107.6	36.5	47.8

Independent value from another reference

445.5	43.14	0	96.84	107.6	43.14	47.9

3*A14+7*A15+3*A18+A19+7*A16+A115+4*A1+3*A2+A3*B3+A30*C30 [326, 415]

$C_{24}H_{37}N_3O$		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]
$C_{24}H_{40}N_8O_4$		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-(*trans*-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-(*trans*-4-pentylcyclohexyl)phenyl]ethanone					
	415.8	34.48	0	82.9	115.5	34.5	48.0

8*A10+2*A12+2*A11+A50+5*A2+A1+A35+A14+3*A15+2*A16 [153]

$C_{25}H_{32}O_2$ 17-phenyl testosterone

388.5	23.3	59.97				
450.0	44.2	98.22	158.2	67.7[a]	67.5	30.5

4*A14+5*A15+3*A17+3*A16+2*A1+A30*B30+A19+A18*B18+A114+
5*A10+A11 [11]

$C_{25}H_{33}O_8$ hydrocortisone hemisuccinate

444.0	41.34	0	93.1	116.2	41.3	51.6

4*A14+5*A15+3*A17+4*A16+2*A1+2*A30*D30+A19+A18*B18+A114+A35+
3*A2+A38+A36*D36 [11]

$C_{25}H_{34}O_3$ 3-[(1-oxoheptyl)oxy]-estra-1,3,5(10)-trien-17-one

338.0	21.0	0	62.1	103.4	21.0	34.9

3*A14+4*A15+2*A19+3*A16+A17+3*A10+A12+A114+A38+2*A1+5*A2 [116]

$C_{25}H_{38}O_5$ Simvastatin

413.8	29.59	0	71.5	119.7	29.6	49.5

3*A14+7*A15+A115+7*A16+3*A18+A19+3*A2+A30*C30+5*A1+A4*B4+A38 [326]

$C_{25}H_{48}N_6O_8$ Deferoxamine

411.1	105.3	0	256.1	210.1	105.3	86.4

A1+19*A2+2*A60+A45+3*A30*D30+3*A59 [89]

$C_{25}H_{50}$ nonadecylcyclohexane

316.2	77.79	0	246.0	214.8	77.79	67.9

A14+3*A15+A1+18*A2*B2+A16 [114]

$C_{25}H_{50}O_2$ methyl tetracosanoate

331.2	90.0	0	271.7	247.5	90.0	81.2

2*A1+A38+22*A2*B2 [245]

$C_{25}H_{52}$ pentacosane

309.0	23.90	77.35				
312.9	1.07	3.42				
325.9	55.53	170.39	251.2	249.1	80.5	81.2

2*A1+23*B2*A2 [351]

$C_{26}H_{15}Cl_2N_5O_2$ 1,3-*bis*(cyano-4-chlorophenylcarbamoyl-methylene)isoindolin [68808-70-8]

679.2	123	0	181.1	102[a]	123	69.3

A14+2*A15+4*A19+A121+12*A10+4*A12+2*A22*D22+2*A56+2*A60+2*A7 [132]

$C_{26}H_{29}NO$ Tamoxifen

371.0	34.0	0	91.6	124.4	34.0	46.2

14*A10+4*A12+3*A2+3*A1+A31+2*A7+A43 [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

A14+3*A15+4*A19+2*A114+4*A10+4*A12+4*A32+4*A1+8*A2 [93]

[Note: The larger tetraalkoxy-derivatives show liquid crystalline behavior]

$C_{26}H_{33}NO_3$ 2-(4-nitrophenyl)-1-[4-[2-(*trans*-4-butylcyclohexyl)ethyl]phenyl]ethanone

408.6	35.90	0	87.86	122.6	35.90	50.1

8*A10+2*A12+2*A11+A50+6*A2+A1+A35+A14+3*A15+2*A16 [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*A1+8*A2+4*A32+6*A10+8*A12 [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*A14+4*A15+2*A19+3*A16+A17+3*A10+A12+A114+A38+2*A1+6*A2 [116]

$C_{26}H_{38}O_2$ 3β-octyloxy-estra-1,3,5(10)-trien-17-one

331.0	19.0	0	57.4	114.6	19.0	37.9

3*A14+4*A15+2*A19+3*A16+A17+3*A10+A12+A114+A32+2*A1+7*A2 [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*A14+4*A15+2*A19+4*A16+A17+3*A10+A12+A32+2*A1+7*A2+A30*B30 [116]

$C_{26}H_{48}N_6O_9$ formamide deferoxamine

430.8	92.93	0	215.7	215.7	92.9	92.9

A1+19*A2+2*A60+3*A30*D30+3*A59+A162 [89]

$C_{26}H_{52}O_2$ methyl pentacosanoate

332.2	92.0	0	276.94	256.8	92.0	85.3

2*A1+A38+23*A2*B2 [245]

$C_{27}H_{19}NO$ 2-phenyl-5-(*p*-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-(*p*-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*H*-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-(*trans*-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-3β-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]

$C_{27}H_{48}N_2OS$ 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]

$C_{27}H_{48}O$ 5α-cholestan-3β-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]
$C_{27}H_{50}N_6O_9$	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-(*p*-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-(*p*-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-*bis*(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]

$C_{28}H_{26}N_4O_8$ 1,4-*bis*(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]

$C_{28}H_{31}FN_4O$ 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]

$C_{28}H_{50}N_6O_{10}S$ 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]

$C_{28}H_{52}N_6O_9$ 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]

$C_{29}H_{26}BCl_2NO_2$ 4-benzhydryl-2,5-di(4'-chlorophenyl)-4,5-dimethyl-1,3-dioxa-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.]

$C_{29}H_{28}BNO_2$ 4-benzhydryl-5,6-dimethyl-2,5-diphenyl-1,3-dioxa-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]

$C_{29}H_{42}O_3$ 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]

$C_{29}H_{44}O_6Si_2$ 4-[[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]

$C_{29}H_{44}O_6Si_2$ 4-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]

$C_{29}H_{51}N_6O_{11}$ 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]

$C_{29}H_{54}N_6O_9$ 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]

$C_{29}H_{58}O_2$ methyl octacosanoate
340.2 109.7 0 322.46 284.7 109.7 96.9
2*A1+A38+26*A2*B2 [245]

$C_{30}H_{22}$ 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]

$C_{30}H_{22}$ 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]

$C_{30}H_{46}F_4O_2$ 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]

$C_{30}H_{56}N_6O_9$ 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-dioxa-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]

$C_{31}H_{58}N_6O_9$ Caproylamide Deferoxamine

450.1	119.2	0	264.8	236.2	119.2	106.3
2*A1+23*A2+2*A60+3*A30*D30+3*A59+A60						[89]

$C_{31}H_{61}AsO_7$ (R)-1,2-dimyristoyloxypropyl-3-arsonic acid

373.7	289.5	0	774.7	312.5[a]	289.5	116.8
2*A1+28*A2*B2+2*A2+2*A38+A3*B3+A181						[94]

$C_{31}H_{61}AsO_7$ (S)-1,2-dimyristoyloxypropyl-3-arsonic acid

374.7	267.8	0	714.7	312.5[a]	267.8	117.1
2*A1+28*A2*B2+2*A2+2*A38+A3*B3+A181						[94]

$C_{31}H_{62}O$ 16-hentricontanone

356.4	117.1	0	328.6	300.2	117.1	107.0
2*A1+28*A2*B2+A35						[297]

$C_{32}H_{38}O_6$ hexa-2,4-diyne-1,6-diyl-*bis*(4-hexyloxybenzoate)

334.2	49.27	0	147.4	157.2	49.3	52.5
2*A1+12*A2+2*A38+4*A9+8*A10+4*A12+2*A32						[115]

$C_{32}H_{41}NO_2$ Terfenadine

422.8	58.1	0	137.4	125.0	58.1	52.9
16*10+4*A11+A14+3*A15+3*A2+3*A1+A3*B3+A4*B4+A16+A119+ 2*A30*C30						[418]

$C_{32}H_{52}N_6O_9$ Benzoylamide Deferoxamine

453.8	107.0	0	235.8	219.7	107.0	99.7
A1+19*A2+2*A60+3*A30*D30+3*A59+A60+5*A10+A12					[89]	

$C_{32}H_{70}Si_{10}$ 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-eicosamethyl-1,10-diphenyl-decasilane

391.2	56.1	0	143.4	139.7	56.1	54.7
10*A109+20*A1+10*A10+2*A12						[183]

$C_{32}H_{66}O$ 17-oxatritriacontane

323.2	10.46	32.36				
324.7	116.73	359.50	391.86	318.9	127.19	103.6
2*A1+A32+30*A2*B2						[189]

$C_{33}H_{30}BNO_2$ 4-benzhydryl-5,6-dimethyl-2-(1'-naphthyl)-5-phenyl-1,3-dioxa-4-aza-2-boracyclohexane

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]

$C_{33}H_{54}N_6O_9$ 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]

$C_{33}H_{62}N_6O_9$ 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*H*-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]

$C_{35}H_{37}N_3O_2$ 4-butoxyphenyl-[6-(4-butoxyphenyl)methyl-9-methyl-9*H*-carbazol-3-yl-methylene)]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]

$C_{35}H_{28}Cl_2N_8O_4$ 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]

$C_{35}H_{50}N_2O_8$ 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]

$C_{36}H_{74}$ hexatricontane

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]

$C_{37}H_{48}N_6O_5S_2$ 2,4,7,12-tetraazatridecan-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-butyoxybenzoyloxy 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]

$C_{39}H_{45}N_3O_2$ 4-hexyloxyphenyl-[6-(4-hexyloxyphenyl)methyl-9-methyl-9*H*-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]

$C_{38}H_{68}S_8$ 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]

$C_{39}H_{78}O$ 20-nonatricontanone

365.6	153.0	0	418.5	374.6	153.0	137.0

2*A1+A35+36*A2*B2 [297]

$C_{39}H_{80}$ 18-butylpentatriacontane

318.5	104.0	0	326.53	355.3	104.0	113.2

3*A1+3*A2+A3+32*A2*B2 [322]

$C_{40}H_{56}$ 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]

$C_{40}H_{82}$ 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

$C_{40}H_{82}$ 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]

$C_{41}H_{44}N_2O_9$ 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]

$C_{41}H_{76}O_8$ 3,5,5-trimethylhexanoic acid, 2,2-*bis*[[(3,5,5-trimethyl-1-oxohexyl)oxy]-

	methyl]-1,3-propanediyl ester					[41058-87-1]
304.0	51.3	0	168.8	158	51.3	48.0
5*A4+4*A38+16*A1+12*A2+4*A3						[50]
$C_{41}H_{84}$	18-hexylpentatricontane					
314.0	107.0	0	340.76	369.5	107.0	116.0
3*A1+5*A2+32*A2*B2+A3						[322]
$C_{42}H_{36}O_{24}S_4$	4-sulfonato-calix[6]arene					
534.8	242.2	0	452.9	122.9[a]	242.2	65.7
6*A145+12*A10+6*A30*D30+A14+21*A15+18*A19						[339]
$C_{42}H_{61}NO_4$	2,7-dihexyloxy-9-(3,5-dihexyloxyphenyl)carbazole					
350.2	41.02	0	117.1	232.6[a]	41.02	81.5
A14+2*A15+4*A19+A119+9*A10+5*A12+4*A32+4*A1+20*A2						
[97]						
$C_{42}H_{86}$	dotetracontane					
344.6	2.11	6.12				
348.6	8.46	24.27				
357.3	165.97	464.51	494.9	407.24	176.54	145.5
40*A2*B2+2*A1						[364]
$C_{43}H_{53}N_3$	4-octylphenyl-[6-(4-octylphenyl)methyl-9-methyl-9*H*-carbazol-3-ylmethylene)]-amine					
425.2	33.1	0	77.85	208.7	33.1	88.7
A14+2*A15+4*A19+14*A10+4*A12+2*A11+2*A6*B6+2*A42+A119+						
3*A1+14*A2						[159]
$C_{44}H_{63}N_3O_2$	2-[3,5-*bis*[4-(dodecyloxy)phenyl]-1*H*-pyrazol-1-yl]pyridine					
344.2	47.3	0	137.42	258.8[a]	47.3	89.1
A14+2*A15+A18+2*A19+A119+A118+12*A10+5*A12+A41+						
2*A32+2*A1+22*A2						[181]
$C_{46}H_{94}$	hexatetracontane					
341.4	23.9	70.01				
360.7	151.4	433.6	503.6	444.4	175.3	160.3
2*A1+44*A2*B2						[296]
$C_{51}H_{69}N_3$	4-dodecylphenyl-[6-(4-dodecylphenyl)methyl-9-methyl-9*H*-carbazol-3-yl-methylene)]amine					

	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]
$C_{52}H_{34}O_2$		1,4-*bis*(2,4,5-triphenylcyclopentadienone-3-yl)benzene					
	594.4	68.8	0	115.8	172.0	68.8	102.2
		2*A14+4*A15+2*A114+8*A19+34*A10+8*A12					[252]
$C_{54}H_{110}$		tetrapentacontane					
	344.9	39.0	113.3				
	368.0	177.2	481.5	594.8	518.9	216.2	190.9
		2*A1+52*A2*B2					[296]
$C_{56}H_{48}O_{32}S_4$		4-sulfonato-calix[8]arene					
	543.1	350.6	0	645.6	96.5[a]	350.6	52.4
		8*A145+A14+29*A15+8*A30*D30+24*A19+16*A10+8*A12					[339]
$C_{57}H_{104}O_6$		1,2,3-tri(*trans*-9-octadecenoyl)glycerol (Trielaidin)					
(I)	314.8	157.07	0	499.0	410.3	157.1	129.2
(II)	288.0	84.20	0	292.4		84.20	
		3*A1+44*A2+A3*B3+3*A38+6*A6					[151]
$C_{57}H_{110}O_6$		tristearin					
(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
		3*A1+48*A2*B2+2*A2 +A3*B3+3*A38					[323]
$C_{58}H_{85}N_3$		4-hexadecylphenyl-[6-(4-hexadecylphenyl)methyl-9-methyl-9*H*-carbazol-3-yl-methylene)]amine					
	405.2	52.1	0	128.6	322.3[a]	52.1	130.6
		A14+2*A15+4*A19+14*A10+4*A12+2*A11+2*A6*B6+2*A42+A119+					
		3*A1+30*A2					[159]
$C_{66}H_{109}NO_4$		2,7-didodecyloxy-9-(3,5-didodecyloxyphenyl)carbazole					
	333.2	61.87	0	185.7	374.6[a]	61.9	124.8
		A14+2*A15+4*A19+A119+9*A10+5*A12+4*A32+4*A1+40*A2					[97]
$C_{72}H_{96}O_{48}$		hexakis(2,3,4-tri-O-acetyl)-α-cyclodextrin					
	505.7	74.37	0	147.1	359.5 [a]	74.4	181.8

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_7S_7 heptasulfur imide

386.7 18.83 0 48.69 18.83

prediction not made [85]

$N_2H_5NO_3$ α-hydrazinium nitrate

138.49 Joules/gram

prediction not made [54]

SeF_2O 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
	Calculation						
$(C_2HClF_3)_n$	poly(chlorotrifluoroethylene)						
	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]

$(C_4H_5ClF_3)_n$ poly(chlorotrifluoroethylene alternate ethylene)

535.0	18.8	0	35.1	25.1	18.8	13.5
2*A4*B4+A22*D22+2*A26*B26+A27+2*A2						[109]

$(C_4H_6O_2)_n$ poly(3-hydroxybutyric acid)

449.0	13.0	0	29.0	22.6	13.0	10.1
A38+A1+A2+A3*B3						[109]

$(C_5H_8)_n$ *trans* polypentenamer

296.0	12.0	0	40.5	38.5	12.0	11.4
3*A2*B2+2*A6						[109]

$(C_5H_9NO)_n$ poly(2,2-dimethyl-3-aminopropanoic acid)

546.0	13.0	0	23.8	20.8	13.0	11.4
A60+A2+A4*B4+2*A1						[109]

$(C_5H_{10})_n$ poly(3-methyl-1-butene)

573.0	17.3	0	30.19	9.5	17.3	5.4
2*A1+2*A3+A2						[109]

$(C_5H_{10}S)_n$ poly(3,3-dimethyltrimethylene sulfide)

292.0	5.23	0	17.9	28.5	5.23	8.3
2*A1+2*A2+A4*B4+A84						[109]

$(C_6H_{10}O_2)_n$ poly(6-hydroxycaproic acid)

337.0	15.4	0	45.7	54.2	15.4	18.3
5*A2*B2+A38						[109]

$(C_6H_{10}O_2)_n$ poly(ε-caprolactone)

?????	11.3	0				
5*A2*B2+A38?						[211]

$(C_6H_{10}O_3)_n$ poly(2,3-dimethyltrimethylene carbonate)

394.2	3.37	0	8.5	9.0	3.4	3.5
2*A1+A2+A3+A3*B3+A149						[249]

$(C_6H_{11}NO_2)_n$ poly(pentamethylene urethane)

415.0	21.0	0	50.6	54.3	21.0	22.5
5*A2*B2+A69						[204]

$(C_6H_{12}O)_n$ poly(hexamethylene oxide)

346.5	23.4	0	67.6	60.5	23.4	21.0
	6*A2*B2+A32					[75]
$(C_6H_{12}S)_n$	poly(hexamethylene sulfide)					
363.3	19.8	0	54.5	57.9	19.8	21.0
	6*A2*B2+A84					[109]
$(C_7H_{13}NO_2)n$	poly(hexamethylene urethane)					
445.0	32.0	0	71.9	63.6	32.0	28.3
	6*A2*B2+A69					[204]
$(C_7H_{14}N_2O)_n$	poly(hexamethylene urea)					
573.0	13.9	0	24.3	47.7	13.9	27.3
	6*A2*B2+A66					[109]
$(C_8H_{12}O_4)_n$	poly(tetramethylene succinate)					
405.2	18.9	0	46.7	66.8	18.9	27.1
	4*A2*B2+2*A2+2*A38					[108]
$(C_8H_{12}O_4)_n$	poly(ethylene adipate					
326.2	21.7	0	66.4	66.8	21.7	21.8
	4*A2*B2+2*A2+2*A38					[101]
$(C_8H_{14})_n$	*cis* polyoctenamer					[52236-40-5]
311.0	21.0	0	67.5	66.4	21.0	20.6
	6*A2*B2+2*A6					[76]
$(C_8H_{14})_n$	*trans* polyoctenamer					
350.0	23.8	0	68.00	66.4	23.8	23.2
	6*A2*B2+2*A6					[109]
$(C_8H_{15}NO)_n$	poly(8-aminocaprylic acid)					
458.0	30.0	0	65.5	66.6	30.0	30.5
	7*A2*B2+A60					[109]
$(C_8H_{16}O)_n$	poly(octamethylene oxide)					
356.0	32.0	0	89.9	79.1	32.0	28.2
	8*A2*B2+A32					[109]
$(C_9H_8O)_n$	alternating copolymer of CO and styrene					
538.0	12.8	0	23.8	31.4	12.8	16.9

	5*A10+A12+A3*B3+A2+A35						[99]
$(C_9H_{14}O_4)_n$	poly(ethylene pimelate)						
	309.2	29.8	0	92.2	76.1	29.8	23.5
	5*A2*B2+2*A2+2*A38						[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*A10+2*A12+2*A38+4*A2+A32						[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*A2*B2+2*A2+2*A38						[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*A2+2*A38+A84						[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*A2+A1+A14+2*A15+2*A16+A18+A19+A131						[337]
$(C_{10}H_{18})_n$	*trans* polydecenamer						
	353.0	32.9	0	93.2	85.0	32.9	26.6
	8*A2*B2+2*A6						[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*A2*B2+2*A60						[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*A2*B2+2*A69						[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

3*A2+2*A38+4*A10+2*A12						[369]
$(C_{11}H_{10}O_4)_n$	poly(trimethylene terephthalate)					
510.0	31.0	0	60.78	51.3	31.0	26.2
3*A2+4*A10+2*A12+2*A30						[41,46]
$(C_{11}H_{18}O_4)_n$	poly(ethylene azelate)					
320.2	43.7	0	136.6	94.7	43.7	30.3
7*A2*B2+2*A2+2*A38						[101]
$(C_{11}H_{18}O_4)_n$	poly(ethylene azelate)					
320.0	43.7	0	136.6	94.7	43.7	30.3
7*A2*B2+2*A2+2*A38						[109]
$(C_{11}H_{21}NO)_n$	poly(11-aminoundecanoic acid)					
493.0	41.0	0	83.2	94.5	41.0	46.6
10*A2*B2+A60						[109]
$(C_{12}H_{16}O_4)_n$	poly(butylene isophthalate)					
429.2	28.0	0	65.2	58.4	28.0	25.1
4*A10+2*A12+2*A38+4*A2						[44]
$(C_{12}H_{22})_n$	*trans* polydodecenamer					
353.0	41.2	0	116.7	103.6	41.2	36.6
10*A2*B2+2*A6						[109]
$(C_{12}H_{22}N_2O_4)_n$	poly(1,4-diisocyanatobutane with 1,6-hexanediol)					
457.0	47.9	0	104.8	108.6	47.9	49.6
10*A2*B2+2*A69						[352]
$(C_{13}H_{24}N_2O_4)_n$	poly(pentamethylene hexamethylenediurethane)					
431.0	42.0	0	97.4	117.9	42.0	50.8
11*A2*B2+2*A69						[109]
$(C_{14}H_{10}O_4)_n$	poly(ethylene 2,6-naphthalate)					
610.0	25.0	0	41.0	44.0	25.0	26.8
2*A2+2*A38+6*A10+4*A12						[109]
$(C_{14}H_{22}O_4)_n$	poly(octamethylene 3-hexenedioate)					
339.0	36.0	0	106.2	114.6	36.0	38.9
8*A2*B2+2*A2+2*A6+2*A38						[109]

$(C_{14}H_{24}N_2O_2)_n$	poly(piperazine sebacamide)					
453.0	26.0	0	57.40	85.5	26.0	38.7
+A14+3*A15+2*A146+8*A2*B2						[109]
$(C_{14}H_{24}O_4)_n$	poly(octamethylene adipate)					
340.0	41.0	0	120.6	127.0	41.0	43.2
12*A2*B2+2*A38						[109]
$(C_{15}H_{28}N_2O_4)_n$	poly(heptamethylene hexamethylenediurethane)					
419.0	48.5	0	115.8	136.5	48.5	57.2
13*A2*B2+2*A69						[109]
$(C_{16}H_{26}O_4)_n$	poly(octamethylene 4-octenedioate)					
312.0	34.0	0	109.0	128.8	34.0	40.2
8*A2*B2+4*A2+2*A6+2*A38						[109]
$(C_{16}H_{26}O_4)_n$	poly(decamethylene 3-hexenedioate)					
339.0	36.0	0	106.2	133.2	36.0	45.2
10*A2*B2+2*A6+2*A2+2*A38						[109]
$(C_{16}H_{30}N_2O_2)_n$	poly(hexamethylene sebacamide)					
501.0	58.6	0	117.0	133.2	58.6	66.7
14*A2*B2+2*A60						[109]
$(C_{16}H_{30}N_2O_4)_n$	poly(octamethylene hexamethylenediurethane)					
430.0	55.2	0	128.4	145.8	55.2	62.7
14*A2*B2+2*A69						[109]
$(C_{17}H_{16}N_2O_4)_n$	poly(ethylene 4,4’-methylenediphenylenediurethane)					
512.0	48.0	0	93.8	61.9	48.0	31.7
3*A2+2*A69+8*A10+2*A11+2*A12						[109]
$(C_{18}H_{24}O_4)_n$	poly(decamethylene terephthalate)					
411.0	46.1	0	112.2	123.0	46.1	50.6
10*A2*B2+2*A38+4*A10+2*A12						[109]
$(C_{18}H_{28}N_2O_4)_n$	poly(decamethylene hexamethylenediurethane)					
427.0	56.5	0	132.3	164.4	56.5	70.2
16*A2*B2+2*A69						[109]

$(C_{18}H_{30}O_4)_n$	poly(decamethylene 4-octenedioate)					
326.0	44.0	0	135.0	147.4	44.0	48.1
10*A2*B2+4*A2+2*A38+2*A6						[109]
$(C_{18}H_{32}O_4)_n$	poly(nonamethylene azelate)					
338.0	49.0	0	145.0	164.2	49.0	55.5
16*A2*B2+2*A38						[109]
$(C_{18}H_{36}N_4)_n$	poly(4,4'-decamethylene dipiperazine)					
403.0	69.1	0	171.5		69.1	
prediction not made						[109]
$(C_{19}H_{35}N_2O_2)_n$	poly(decamethylene azelamide)					
487.0	68.2	0	140.0	161.1	68.2	78.5
17*A2*B2+2*A60						[109]
$(C_{20}H_{34}O_4)_n$	poly(tetradecamethylene 3-hexenedioate)					
353.0	49.0	0	138.8	170.4	49.0	60.2
14*A2*B2+2*A2+2*A6+2*A38						[109]
$(C_{20}H_{36}O_4)_n$	poly(tetradecamethylene adipate)					
353.0	59.0	0	167.14	182.8	59.0	64.5
18*A2*B2+2*A38						[109]
$(C_{20}H_{38}N_2O_2)_n$	poly(decamethylene sebacamide)					
471.0	72.0	0	152.9	170.4	72.0	80.3
18*A2*B2+2*A60						[109]
$(C_{21}H_{22}O_4)_n$	poly(heptane-1,7-diyl biphenyl-4,4'-dicarboxylate)					
438.0	10.8	0	24.7	94.3[a]	10.8	41.3
7*A2+2*A38+8*A10+4*A12						[256]
$(C_{21}H_{24}N_2O_4)_n$	poly(hexamethylene 4,4'-methylenediphenylenediurethane)					
462.0	52.0	0	112.6	94.5	52.0	43.7
7*A2+2*A69+8*A10+4*A12						[109]
$(C_{22}H_{26}N_2O_4)_n$	poly(heptamethylene 4,4'-methylenediphenylenediurethane)					
471.0	50.6	0	107.4	101.6	50.6	47.9
8*A2+2*A69+8*A10+4*A12						[109]
$(C_{22}H_{38}O_4)_n$	poly(tetradecamethylene 4-octenedioate)					

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]

$(C_{24}H_{28}N_2O_4)_n$ 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]

$(C_{25}H_{30}N_2O_4)_n$ 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]

$(C_{26}H_{50}N_2O_2)_n$ poly(tridecamethylene tridecanediamide)

456.0	97.2	0	213.2	226.2	97.2	103.2
24*A2*B2+2*A60						[109]

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$C_{40}H_{76}Si_5$ $Si[CH_2CH_2CH_2Si(CH_3)[CH_2CH{=}CH_2)_2]_4$

222.8	39.2	0	176	257.6[a]	39.2	57.4
A109+4*(A109+5*A2+2*A6+2*A5+A1)						[64]

$C_{168}H_{364}O_{24}Si_{21}$ $Si\{CH_2CH_2CH_2Si(CH_3)[CH_2CH_2CH_2Si(CH_3)_2OSi(CH_3)_2(CH_2)_{10}\text{-}COOCH_3]_2\}_4$

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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