#920208A1

PRIVILEGED DOCUMENT
FOR REVIEW PURPOSES ONLY

Supplemental Tables

Group Values for Estimating Heat Capacities of Liquids and Solids

Hydrocarbon Groups	Benson Notation[a]	Group Values[b,c] $C_p(l)$ J/(K mole)	$C_p(c)$ J/(K mole)	data points liquids	solids
primary sp^3 carbon	$C(H)_3-(C)$	34.9	36.6	25	14
secondary sp^3 carbon	$C(H)_2-(C)_2$	31.9	26.9	24	14
tertiary sp^3 carbon	$C(H)-(C)_3$	22.4	9.00	20	11
quaternary sp^3 carbon	$C-(C)_4$	14.0	-4.98	17	7
secondary sp^2 carbon	$C_d(H)_2$	25.8	[46.0]	18	3
tertiary sp^2 carbon	$C_d(H)-(C)$	27.8	21.4	22	13
quaternary sp^2 carbon	$C_d-(C)_2$	21.7	[6.86]	30	6
tertiary sp carbon	$C_t(H)$	[34.3]	[37.1]	3	3
quaternary sp carbon	$C_t-(C)$, and C_a	28.9	[15.5]	9	6
tertiary aromatic sp^2 carbon	$C_B(H)$	21.8	17.5	32	27
quaternary aromatic sp^2 carbon	$C_{BF}(C_B)_2(C_{BF})$, and $C_{BF}(C_B)(C_{BF})_2$, and $C_B-(C)$	15.3	8.49	32	27
internal quaternary aromatic sp^2 carbon	$C_{BFi}(C_{BF})_3$	16.0	~~[4.44]~~ 9.1		4
cyclic secondary sp^3 carbon	$C_c(H)_2-(C_c)_2$	25.9	24.6	46	27
cyclic tertiary sp^3 carbon	$C_c(H)-(C_c)_2(C)$	20.6	11.7	40	20
cyclic quaternary sp^3 carbon	$C_c-(C_c)_2(C)_2$	18.0	6.11	12	11
cyclic tertiary sp^2 carbon	$C_{cd}(H)-(C_c)$	21.8	15.9	17	7
cyclic quaternary sp^2 carbon	$C_{cd}-(C_c)(C)$	21.2	[4.73]	12	5

[a] the subscripts used in this column follow the notation used by Benson and have the following meanings: d: double bond; t: triple bond; B: carbon atom in benzene and related heterocycles; a: allenic carbon; BF: a carbon atom in a fused ring system such as naphthalene and $C_{BFi}-(C_{BF})_3$ represents a carbon atom in a graphite environment such as found in the two internal carbons of perylene (see text); subscript c refers to ring atoms (not used by the Benson notation); unsubscripted carbon atoms may be C_d, C_B, C_t, C_C, C_{Cd} or any one of the functional groups listed in Table II; C_{cd} and C_B groups may be substituted for the C_c group; groups that potentially can be varied are set off by a hyphen; see text for further discussion; 1 cal = 4.184 J.

[b] values in brackets are considered as tentative assignments only.

[c] there are no other corrections to be applied.

1/8/9

Table II Functional Group Values for Estimating Heat Capacities of Liquids and Solids at 298 K

Functional Group	Benson Notation[a]	Group Values[b] Cp(l) J/(K mole)	Cp(c)	data points liquids	solids
hydroxyl	HO-(C)	53.1	23.5	73	33
fluorine	F-(C)	16.2	[24.8]	46	4
chlorine	Cl-(C)	30.8	28.7	37	17
bromine	Br-(C)	34.6	32.4	26	9
iodines	I-(C)	39.1	[27.9]	8	3
nitrile	NC-(C)	47.7	[42.3]	17	8
carboxylic acid	CO(OH)-(C)	87.4	53.1	13	35
acid chloride	CO(Cl)-(C)	[62.8]	[60.2]	4	1
aldehyde	CO(H)-(C)	57.7	[84.5]	19	2
ketones	CO-$(C)_2$	51.5	[28.0]	23	5
cyclic ketones	CO-$(C_c)_2$	[46.4]	34.3	3	8
ester	CO_2-$(C)_2$	63.2	40.3	72	24
lactone	CO_2-$(C_c)_2$	[67.4]	[45.2]	4	5
cyclic carbonates	CO_3-$(C_c)_2$	[92.0]	[68.2]	5	1
cyclic anhydrides	CO_2CO-$(C_c)_2$		[80.3]		6
ether	O-$(C)_2$	29.8	49.8	54	8
cyclic ether	O-$(C_c)_2$	24.6	9.71	20	16
isocyanate	OCN-(C)	[58.2]	[52.7]	5	3
nitro group	O_2N-(C)	[58.6]	56.1	6	26
thiols	HS-(C)	49.0	[51.9]	23	1
primary sp^3 nitrogen	$N(H)_2$-(C)	59.4	21.6	21	38
secondary sp^3 nitrogen	N(H)-$(C)_2$	[51.0]	[-0.29]	6	3
tertiary sp^3 nitrogen	N-$(C)_3$	22.0	[31.5]	10	2
tertiary sp^2 nitrogen	$N_I(H)$-(C_d), and $N_A(H)$-(C_d)	[44.4]	10.7	3	10
cyclic secondary sp^3 nitrogen	N(H)-$(C_c)_2$	46.0	23.9	11	9
cyclic tertiary sp^3 nitrogen	N-$(C_c)_2$(C)	[28.6]	1.21	6	7
cyclic tertiary sp^2 nitrogen	N_d-$(C_{cd})(C_c)$, and N_d-$(C_B)_2$	20.7	13.9	12	9
primary amides	$CO(NH_2)$-(C)	[41.0]	[54.4]	1	4
secondary amide	CONH-$(C)_2$	79.9	44.4	9	13
tertiary amides	CON-$(C)_3$	[82.4]		1	
cyclic secondary amide	CONH-$(C_c)_2$	[92.0]	46.4	1	9
cyclic tertiary amide	CON-$(C_c)_2$(C)	[170]	[52.7]	1	3
carbamates	$NHCO_2$-$(C)_2$		[76.1]		4
cyclic imide	$NH(CO)_2$-$(C_c)_2$		[74.1]		2
mono substituted ureas	NH_2CONH-(C)		[82.8]		3
cyclic urea	$CO(NH)_2$-$(C_c)_2$		[63.6]		1
mono substituted guanidine group	$NH_2(C{=}NH)NH$-(C)		[59.4]		2
sulfides	S-$(C)_2$	40.3	[116]	14	1
cyclic sulfides	S-$(C_c)_2$	33.8	[20.3]	11	1
disulfides	S_2-$(C)_2$	[74.5]	[41.0]	2	1
sulfoxides	SO-$(C)_2$	[83.7]	[47.7]	1	1
sulfones	SO_2-$(C)_2$		[88.7]		1
sulfonamides	SO_2NH_2-(C)		[104]		2

Table II [Continued]

Functional Groups	Benson Notation[ac]	Group Values[b] $C_p(l)$ J/(K mole)	Group Values[b] $C_p(c)$ J/(K mole)	data points liquids	data points solids
quaternary silicon	$Si-(C^*)_4$	30.9	32.4	24	16
tertiary aluminum	$Al-(C^*)_3$	[46.9]		3	
quaternary tin	$Sn-(C^*)_4$	[58.6]	[77.2]	1	2
quaternary germanium	$Ge-(C^*)_4$	[48.1]	[18.9]	1	2
phosphine oxide	$PO-(C^*)_3$		[28.5]		1

[a] N_I and N_A refer to imino and azo nitrogens, respectively.
[b] values in brackets are considered as tentative assignments only.
[c] due to insufficient experimental data, only the parameters listed in Table I can be substituted for a C*.

Liquid Linear Hydrocarbons*

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc***
C_2H_6	ethane	74.5	69.9	4.6
C_3H_8	propane	98.3	101.7	-3.4
C_4H_{10}	butane	132.6	133.5	-0.9
C_5H_{12}	pentane	168.2	165.3	2.9
C_6H_{14}	n-hexane	198.3	197.1	1.2
C_7H_{16}	heptane	224.7	229.3	-4.6
C_8H_{18}	n-octane	254.0	261.1	-7.1
C_9H_{20}	nonane	284.1	292.9	-8.8
$C_{10}H_{22}$	n-decane	314.6	324.7	-10.1
$C_{11}H_{24}$	n-undecane	345.2	356.5	-11.3
$C_{12}H_{26}$	dodecane	376.1	388.7	-12.6
$C_{13}H_{28}$	tridecane	407.1	420.5	-13.4
$C_{14}H_{30}$	tetradecane	438.9	452.3	-13.4
$C_{15}H_{32}$	n-pentadecane	469.9	484.1	-14.2
$C_{16}H_{34}$	hexadecane	504.2	515.9	-11.7
$C_{17}H_{36}$	n-heptadecane	534.3	548.1	-13.8
$C_{18}H_{38}$	octadecane	564.4	579.9	-15.5
$C_{20}H_{42}$	eicosane	663.6	643.5	20.1
$C_{22}H_{46}$	n-docosane	740.6	707.5	33.1
$C_{23}H_{48}$	tricosane	774.0	739.3	34.7
$C_{26}H_{54}$	n-hexacosane	870.3	834.7	35.6
$C_{28}H_{58}$	octacosane	937.2	898.7	38.5
$C_{32}H_{66}$	dotriacontane*	1355.6	1025.9	
$C_{33}H_{68}$	triatriacontane	1112.5	1058.1	54.4
$C_{36}H_{74}$	hexatriacontane	1205.0	1153.5	51.5
$C_{48}H_{98}$	octatetracontane	1594.1	1536.4	57.7

* not used in the correlation
** the group values listed below were evaluated in the same sequence as they appear in this table
*** discrepancies in differences between calculated and experimental are due to rounding errors

Parameters derived from the correlation:	Group	Entries
primary sp^3 carbon (1):	34.9	25
secondary sp^3 carbon (1):	31.9	24

Liquid Branched Saturated Hydrocarbons

	Compounds	Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_6H_{14}	2,3-dimethylbutane	188.7	184.1	4.6
C_6H_{14}	3-methylpentane	190.8	190.8	0.0
C_6H_{14}	2-methylpentane	193.7	190.8	2.9
C_7H_{16}	2,4-dimethylpentane	224.3	216.3	8.0
C_7H_{16}	2,3-dimethylpentane	215.9	216.3	-0.4
C_7H_{16}	3-ethylpentane	219.7	222.6	-2.9
C_7H_{16}	3-methylhexane	214.2	222.6	-8.4
C_7H_{16}	2-methylhexane	223.0	222.6	0.4
C_8H_{18}	2,5-dimethylhexane	249.4	248.1	1.3
C_8H_{18}	2,3,4-trimethylpentane	247.3	241.4	5.9
C_8H_{18}	4-methylheptane	251.0	254.4	-3.4
C_8H_{18}	3-methylheptane	249.8	254.4	-4.6
C_8H_{18}	2-methylheptane	251.9	254.4	-2.5
$C_{10}H_{22}$	2,7-dimethyloctane	301.7	311.7	-10.0
$C_{10}H_{22}$	5-methylnonane	314.6	318.4	-3.8
$C_{10}H_{22}$	(DL)4-methylnonane	317.6	318.4	-0.8
$C_{10}H_{22}$	(DL)3-methylnonane	309.2	318.4	-9.2
$C_{10}H_{22}$	2-methylnonane	313.4	318.4	-5.0
$C_{11}H_{24}$	2-methyldecane	341.4	350.2	-8.8
$C_{31}H_{64}$	11-n-decylheneicosane	949.8	987.4	-37.6

Parameter derived from the correlation:	Group	Entries
tertiary sp^3 carbon (1):	22.4	20

Liquid Cycloalkanes

	Compounds	Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_3H_6	cyclopropane	81.2	77.4	3.8
C_4H_8	cyclobutane	106.3	103.3	3.0
C_5H_{10}	cyclopentane	128.9	129.3	-0.4
C_6H_{12}	cyclohexane	156.1	155.2	0.9
C_7H_{14}	cycloheptane	180.7	181.2	-0.5
C_8H_{16}	cyclooctane	215.5	206.7	8.8
C_6H_{12}	methylcyclopentane	158.6	159.0	-0.4
C_7H_8	quadricyclane	157.7	149.8	7.9
C_7H_{12}	*cis* bicyclo[4.1.0]heptane	187.9	170.7	17.2
C_7H_{14}	*cis* 1,2-dimethylcyclopentane	190.8	188.7	2.1
C_7H_{14}	*trans* 1,3-dimethylcyclopentane	190.8	188.7	2.1
C_7H_{14}	ethylcyclopentane	187.4	190.8	-3.4
C_7H_{14}	methylcyclohexane	184.5	184.9	-0.4
C_8H_{14}	*trans* bicyclo[3.3.0]octane	180.3	196.2	-15.9

C_8H_{14}	*cis* bicyclo[3.3.0]octane	213.4	196.2	17.2
C_8H_{14}	*cis* bicyclo[4.2.0]octane	258.6	196.2	62.4
C_8H_{14}	*endo*-2-methylbicyclo[2.2.1] heptane	184.1	200.0	-15.9
C_8H_{14}	*exo*-2-methylbicyclo[2.2.1] heptane	185.8	200.0	-14.2
C_8H_{16}	propylcyclopentane	216.3	222.6	-6.3
C_8H_{16}	*trans* 1,2-dimethylcyclohexane	209.6	214.2	-4.6
C_8H_{16}	*cis* 1,2-dimethylcyclohexane	210.0	214.2	-4.2
C_8H_{16}	*trans* 1,3-dimethylcyclohexane	213.0	214.2	-1.2
C_8H_{16}	*cis* 1,3-dimethylcyclohexane	209.2	214.2	-5.0
C_8H_{16}	*trans* 1,4-dimethylcyclohexane	210.5	214.2	-3.7
C_8H_{16}	*cis* 1,4-dimethylcyclohexane	212.1	214.2	-2.1
C_8H_{16}	ethylcyclohexane	211.7	216.7	-5.0
C_9H_{16}	*cis* bicyclo[6.1.0]nonane	235.1	222.2	12.9
C_9H_{16}	*trans* hexahydroindane	209.6	222.2	-12.6
C_9H_{16}	*cis* hexahydroindane	214.2	222.2	-8.0
C_9H_{18}	n-butylcyclopentane	245.2	254.4	-9.2
C_9H_{18}	n-propylcyclohexane	242.3	248.5	-6.2
$C_{10}H_{16}$	*exo*-tetrahydrodicyclopentadiene	236.4	237.7	-1.3
$C_{10}H_{18}$	*cis* bicyclo[5.3.0]decane	311.3	248.1	63.2
$C_{10}H_{18}$	*cis* decalin	232.2	248.1	-15.9
$C_{10}H_{18}$	*trans* decalin	228.4	248.1	-19.7
$C_{10}H_{18}$	bicyclopentyl	238.9	248.1	-9.2
$C_{10}H_{20}$	n-butylcyclohexane	271.1	280.3	-9.2
$C_{12}H_{22}$	bicyclohexyl	282.8	300.0	-17.2
$C_{13}H_{26}$	n-heptylcyclohexane	363.2	376.1	-12.9
$C_{15}H_{30}$	n-decylcyclopentane	426.3	446.0	-19.7
$C_{16}H_{32}$	n-decylcyclohexane	455.6	471.5	-15.9
$C_{18}H_{36}$	n-dodecylcyclohexane	615.5	535.6	79.9
$C_{18}H_{36}$	hexaethylcyclohexane	530.1	524.3	5.8
$C_{25}H_{46}$	4'-n-heptyl-m-tercyclohexyl	668.6	665.3	3.3
$C_{25}H_{46}$	4'-n-heptyl-p-tercyclohexyl	752.7	665.3	87.4
$C_{26}H_{52}$	11-cyclohexyleicosane	787.4	784.1	3.3

Parameters derived from the correlation:	Group	Entries
cyclic secondary sp^3 carbon (1):	25.9	46
cyclic tertiary sp^3 carbon (1):	20.6	40

Liquid Acyclic Alkenes

	Compounds	Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_3H_8	propene	102.1	88.3	13.8
C_4H_6	1,3-butadiene	123.8	106.7	17.1
C_4H_8	1-butene	118.0	120.1	-2.1
C_4H_8	*cis* 2-butene	127.2	125.1	2.1
C_4H_8	*trans*-2-butene	124.3	125.1	-0.8
C_5H_8	*cis* 1,3-pentadiene	146.4	143.9	2.5
C_5H_8	*trans* 1,3-pentadiene	149.4	143.9	5.5
C_5H_8	1,4-pentadiene	146.9	138.5	8.4

C_5H_{10}	*cis* 2-pentene	147.7	157.3	-9.6
C_5H_{10}	*trans* 2-pentene	156.9	157.3	-0.4
C_5H_{10}	1-pentene	155.2	151.9	3.3
C_5H_{10}	3-methyl-1-butene	156.1	145.6	10.5
C_6H_{10}	1,5-hexadiene	133.1	170.7	-37.6
C_6H_{12}	1-hexene	183.3	184.1	-0.8
C_7H_{14}	1-heptene	211.7	215.9	-4.2
C_8H_{14}	allylcyclopentane	202.9	209.2	-6.3
C_8H_{16}	1-octene	241.4	247.7	-6.3
C_9H_{16}	allylcyclohexane	233.5	235.1	-1.6
$C_{10}H_{20}$	1-decene	300.4	311.3	-10.9
$C_{11}H_{22}$	1-undecene	330.1	343.5	-13.4
$C_{12}H_{24}$	1-dodecene	360.7	375.3	-14.6
$C_{16}H_{32}$	1-hexadecene	484.9	502.9	-18.0

Parameters derived from the correlation:	Group	Entries
secondary sp^2 carbon (1):	25.8	18
tertiary sp^2 carbon (1):	27.8	22

Liquid Aromatic Hydrocarbons

	Compounds	Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_6H_6	benzene	136.4	131.0	5.4
C_7H_8	toluene	156.9	159.0	-2.1
C_8H_8	styrene	182.8	177.8	5.0
C_8H_{10}	o-xylene	187.9	187.4	0.5
C_8H_{10}	m-xylene	183.3	187.4	-4.1
C_8H_{10}	p-xylene	183.7	187.4	-3.7
C_8H_{10}	ethylbenzene	185.8	191.2	-5.4
C_9H_{10}	indane	190.4	195.4	-5.0
C_9H_{12}	1,2,3-trimethylbenzene	216.3	215.9	0.4
C_9H_{12}	1,2,4-trimethylbenzene	215.1	215.9	-0.8
C_9H_{12}	1,3,5-trimethylbenzene	209.2	215.9	-6.7
C_9H_{12}	isopropylbenzene	215.5	216.3	-0.8
C_9H_{12}	n-propylbenzene	214.6	223.0	-8.4
$C_{10}H_{12}$	1,2,3,4-tetrahydronaphthalene	217.6	221.3	-3.7
$C_{10}H_{14}$	1,2,3,4-tetramethylbenzene	236.0	244.3	-8.3
$C_{10}H_{14}$	1,2,3,5-tetramethylbenzene	240.2	244.3	-4.1
$C_{10}H_{14}$	1-isopropyl-4-methylbenzene	236.4	244.8	-8.4
$C_{10}H_{14}$	n-butylbenzene	243.5	254.8	-11.3
$C_{11}H_{10}$	1-methylnaphthalene	224.3	233.5	-9.2
$C_{11}H_{10}$	2-methylnaphthalene	228.0	233.5	-5.5
$C_{12}H_{10}$	biphenyl	300.0	248.5	51.5
$C_{12}H_{18}$	hexamethylbenzene	370.7	300.8	69.9
$C_{13}H_{12}$	diphenylmethane	266.1	280.3	-14.2
$C_{14}H_{12}$	1,2-diphenylethylene	343.1	304.2	38.9
$C_{14}H_{14}$	2,2'-dimethylbiphenyl	297.9	305.4	-7.5
$C_{14}H_{14}$	2-ethylbiphenyl	302.9	308.8	-5.9
$C_{14}H_{14}$	1,2-diphenylethane	320.1	312.5	7.6
$C_{14}H_{14}$	1,2,3,4-tetrahydrophenanthrene	278.2	295.4	-17.2
$C_{15}H_{16}$	p-isopropylbiphenyl	343.9	334.3	9.6
$C_{18}H_{14}$	o-terphenyl	369.0	366.5	2.5

$C_{18}H_{14}$	m-terphenyl	417.1	366.5	50.6
$C_{24}H_{34}$	1,1-diphenyldodecane	593.7	624.7	-31.0
$C_{24}H_{46}$	1-phenyl-1-cyclohexyldodecane	610.9	650.2	-39.3

Parameters derived from the correlation:	Group	Entries
tertiary aromatic sp^2 carbon (l):	21.8	32
quaternary aromatic sp^2 carbon (l):	15.3	32

Liquid Branched Hydrocarbons with Quaternary Centers

	Compounds	Heat Capacities J/(K mole) C_p(l) Expt	C_p(l) Calc	Expt-Calc
C_5H_{12}	2,2-dimethylpropane	153.1	153.6	-0.5
C_6H_{14}	2,2-dimethylbutane	188.7	185.4	3.3
C_6H_{12}	3,3-dimethyl-1-butene	188.3	172.0	16.3
C_7H_{16}	3,3-dimethylpentane	211.7	217.1	-5.4
C_7H_{16}	2,2,3-trimethylbutane	213.4	210.9	2.5
C_7H_{16}	2,2-dimethylpentane	221.3	217.1	4.2
C_8H_{18}	2,2,4-trimethylpentane	238.9	242.7	-3.8
C_8H_{18}	3,3-dimethylhexane	246.4	248.9	-2.5
C_8H_{18}	2,2,3-trimethylpentane	245.6	242.7	2.9
C_8H_{18}	isooctane	241.0	242.7	-1.7
C_9H_{20}	2,2,3,3-tetramethylpentane	271.5	269.0	2.5
C_9H_{20}	2,2,4,4-tetramethylpentane	266.5	269.0	-2.5
C_9H_{20}	3,3-diethylpentane	278.2	280.7	-2.5
$C_{10}H_{14}$	t-butylbenzene	238.1	242.7	-4.6
$C_{10}H_{20}$	t-butylcyclohexane	264.8	268.6	-3.8
$C_{12}H_{26}$	2,2,4,6,6-pentamethylheptane	351.0	358.2	-7.2
$C_{16}H_{34}$	2,2,4,4,6,8,8-heptamethylnonane	459.0	473.6	-14.6

Parameter derived from the correlation:	Group	Entries
quaternary sp^3 carbon (l):	14.0	17

Liquid Cyclic Olefins

	Compounds	Heat Capacities J/(K mole) C_p(l) Expt	C_p(l) Calc	Expt-Calc
C_5H_6	cyclopentadiene	115.5	113.4	2.1
C_5H_8	cyclopentene	122.6	121.3	1.3
C_6H_8	1,3-cyclohexadiene	144.8	138.9	5.9
C_6H_8	1,4-cyclohexadiene	146.0	138.9	7.1
C_6H_{10}	cyclohexene	149.4	147.3	2.1
C_6H_{10}	3-methylcyclopentene	152.3	151.0	1.3
C_7H_8	cycloheptatriene	162.8	156.9	5.9
C_7H_8	norbornadiene	161.1	154.4	6.7
C_7H_{12}	*cis* cycloheptene	171.5	172.8	-1.3
C_7H_{12}	4-methylcyclohexene	180.3	176.6	3.7
C_8H_8	cyclooctatetraene	185.4	174.9	10.5
C_8H_{12}	1,5-cyclooctadiene	198.7	190.8	7.9
C_8H_{12}	2-bicyclo[2.2.2]octene	156.9	188.3	-31.4

C_4H_8	isobutene	121.3	117.2	4.1
C_4H_8O	2-methoxy-1-propene	162.3	146.9	15.4
$C_5H_4O_2$	furfural	162.8	169.0	-6.2
C_5H_6O	2-methylfuran	143.9	111.3	32.6
$C_5H_6O_2$	furfuryl alcohol	215.5	196.2	19.3
C_5H_6S	2-methylthiophene	149.8	155.2	-5.4
C_5H_8	methylenecyclobutane	131.0	124.7	6.3
C_5H_8	2-methyl-1,3-butadiene	152.7	136.0	16.7
$C_5H_8O_2$	acetylacetone (enol)	208.4	223.8	-15.4
$C_5H_8O_2$	methyl 2-methylpropenoate	188.7	180.3	8.4
C_5H_{10}	2-methyl-2-butene	152.7	154.0	-1.3
C_5H_{10}	2-methyl-1-butene	157.3	149.0	8.3
C_6H_7N	1-cyano-3-methylene-cyclobutane	190.8	166.9	23.9
C_6H_8S	2,5-dimethylthiophene	178.2	189.5	-11.3
C_6H_9N	2,4-dimethylpyrrole	192.0	201.7	-9.7
C_6H_9N	2,5-dimethylpyrrole	195.4	201.7	-6.3
C_6H_{10}	1-methylcyclopentene	153.1	155.6	-2.5
$C_6H_{10}O$	4-methylpenten-3-one	187.9	205.4	-17.5
C_6H_{12}	2,3-dimethyl-2-butene	174.9	182.8	-7.9
C_7H_{12}	1-ethylcyclopentene	188.3	187.4	0.9
C_7H_{12}	ethylidenecyclopentane	181.2	187.4	-6.2
C_7H_{12}	methylenecyclohexane	177.4	176.1	1.3
C_8H_{14}	ethylidenecyclohexane	203.8	213.0	-9.2
$C_8H_{14}O$	6-methyl-5-hepten-2-one	268.6	269.4	-0.8
$C_8H_{14}O_2$	butyl methacrylate	273.6	276.1	-2.5
C_9H_{10}	α-methylstyrene	202.1	206.7	-4.6
$C_{10}H_{16}$	limonene	249.4	258.6	-9.2
$C_{10}H_{16}O$	3,7-dimethyl-6-octen-1-yn-3-ol	385.3	348.1	37.2
$C_{10}H_{16}O$	pulegone	274.9	292.0	-17.1
$C_{10}H_{16}O$	citral	304.6	325.1	-20.5
$C_{10}H_{18}O$	2,6-dimethyl-2,7-octadien-6-ol	372.4	338.5	33.9
$C_{12}H_{22}O_2$	octyl methacrylate	386.2	403.3	-17.1
$C_{13}H_{15}NO$	1-(1-isocyanato-1-methylethyl 3-(1-methylethenyl)benzene	382.0	341.8	40.2
$C_{13}H_{20}O$	6,10-dimethyl-3,5,9-undecatrien-2-one	413.4	409.2	4.2
$C_{14}H_{26}O_2$	decyl methacrylate	452.7	467.4	-14.7
$C_{18}H_{32}O$	6,10,14-trimethyl-3,5-pentadecadien-2-one	555.2	566.9	-11.7

Parameters derived from the correlation:	Group	Entries
quaternary sp^2 carbon (l):	21.7	30
cyclic quaternary sp^2 carbon (l):	21.2	12

Mixed Functional Groups Used to Evaluate Liquid Hydrocarbon Parameters

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_4F_8	octafluorocyclobutane	209.6	201.7	7.9
C_5H_5N	1-cyanobicyclobutane	131.8	138.1	-6.3

$C_5H_6Cl_2O$	3,3-bis-(chloromethyl)-oxacyclobutane	218.8	219.7	-0.9
$C_6H_8O_2$	methyl bicyclobutane-1-carboxylate	192.9	188.3	4.6
C_7F_{14}	perfluoromethylcyclohexan	353.1	349.4	3.7
C_7H_9N	1-cyanobicyclo[3.1.0] hexane	170.3	190.0	-19.7
C_7H_{14}	1,1-dimethylcyclopentane	187.4	191.2	-3.8
C_8H_{16}	1,1-dimethylcyclohexane	209.2	217.1	-7.9
$C_{10}H_{18}$	pinane	231.8	261.9	-30.1
$C_{10}F_{14}$	perfluorobicyclo[4.4.0] deca-1,6-diene	428.4	420.1	8.3
$C_{10}F_{18}$	*cis* perfluorodecalin	449.8	472.0	-22.2
$C_{10}F_{18}$	*trans* perfluorodecalin	446.9	472.0	-25.1

Parameter derived from the correlation:	Group	Entries
cyclic quaternary sp^3 carbon (1):	18.0	12

Functional Group Parameters-Liquids

Liquid Alcohols

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
CH_4O	methanol	81.6	87.9	-6.3
C_2H_6O	ethanol	111.7	120.1	-8.4
$C_2H_6O_2$	dihydroxyethane	166.9	169.9	-3.0
C_3H_6O	propenol	138.9	138.5	0.4
$C_3H_6O_3$	*dl*-lactic acid	210.5	197.9	12.6
C_3H_8O	1-propanol	140.2	151.9	-11.7
C_3H_8O	2-propanol	149.8	145.2	4.6
$C_3H_8O_2$	1,2-dihydroxypropane	180.3	195.4	-15.1
$C_3H_8O_3$	1,2,3-trihydroxypropane	223.4	245.6	-22.2
$C_4H_{10}O$	isobutyl alcohol	180.7	177.0	3.7
$C_4H_{10}O$	butyl alcohol	177.0	183.7	-6.7
$C_4H_{10}O$	2-butanol	197.5	177.0	20.5
$C_4H_{10}O$	t-butyl alcohol	218.4	171.5	46.9
$C_4H_{10}O2$	1,3-butanediol	227.2	223.0	4.2
$C_4H_8O_2$	1,4-butanediol	200.0	233.9	-33.9
$C_4H_8O_2$	2,3-butanediol	213.0	220.9	-7.9
$C_5H_{10}O$	2-methyl-3-buten-2-ol	208.4	190.4	18.0
$C_5H_{12}O$	2-methyl-2-butanol	247.3	203.8	43.5
$C_5H_{12}O$	3-methyl-1-butanol	209.6	209.2	0.4
$C_5H_{12}O$	2,2-dimethyl-1-propanol	244.3	203.8	40.5
$C_5H_{10}O$	cyclopentanol	185.4	177.4	8.0
$C_5H_{12}O$	3-pentanol	239.7	209.2	30.5
$C_5H_{12}O$	1-pentanol	208.4	215.5	-7.1
$C_6H_{12}O$	cyclohexanol	213.4	202.9	10.5
$C_6H_{14}O$	3-hexanol	286.2	241.0	45.2
$C_6H_{14}O$	2-methyl-1-pentanol	248.5	241.0	7.5
$C_6H_{14}O$	3-methyl-3-pentanol	293.3	235.6	57.7
$C_6H_{14}O$	4-methyl-2-pentanol	273.2	234.3	38.9

$C_6H_{14}O$	3-methyl-2-pentanol	275.7	234.3	41.4
$C_6H_{14}O$	1-hexanol	242.7	247.3	-4.6
C_7H_8O	benzyl alcohol	215.9	209.2	6.7
$C_7H_{14}O$	3-methylcyclohexanol	199.6	232.6	-33.0
$C_7H_{14}O$	4-methylcyclohexanol	202.1	232.6	-30.5
$C_7H_{14}O$	2-methylcyclohexanol	199.6	232.6	-33.0
$C_7H_{14}O$	cycloheptanol	250.2	228.9	21.3
$C_7H_{16}O$	1-heptanol	270.7	279.5	-8.8
$C_8H_{10}O$	2-phenylethanol	252.7	241.4	11.3
$C_8H_{18}O$	5-methyl-1-heptanol	304.2	304.6	-0.4
$C_8H_{18}O$	1-octanol	312.1	311.3	0.8
$C_8H_{18}O$	2-octanol	330.1	304.6	25.5
$C_8H_{18}O$	3-octanol	338.5	304.6	33.9
$C_8H_{18}O$	4-octanol	337.6	304.6	33.0
$C_8H_{18}O$	2-ethylhexanol	317.6	304.6	13.0
$C_8H_{18}O$	2-methyl-1-heptanol	313.0	304.6	8.4
$C_8H_{18}O$	2-methyl-4-heptanol	331.8	298.3	33.5
$C_8H_{18}O$	2-methyl-2-heptanol	337.6	299.2	38.4
$C_8H_{18}O$	3-methyl-2-heptanol	297.5	298.3	-0.8
$C_8H_{18}O$	4-methyl-2-heptanol	312.5	298.3	14.2
$C_8H_{18}O$	4-methyl-3-heptanol	309.2	298.3	10.9
$C_8H_{18}O$	4-methyl-4-heptanol	367.4	299.2	68.2
$C_8H_{18}O$	5-methyl-2-heptanol	296.2	298.3	-2.1
$C_8H_{18}O$	6-methyl-2-heptanol	315.1	298.3	16.8
$C_8H_{18}O$	6-methyl-3-heptanol	310.5	298.3	12.2
$C_9H_{12}O$	3-phenylpropanol	280.7	273.2	7.5
$C_{10}H_{16}O$	3,7-dimethyl-6-octen-1-yn-3-ol	385.3	348.1	37.2
$C_{10}H_{18}O$	2,6-dimethyl-2,7-octadien-6-ol	372.4	338.5	33.9
$C_{10}H_{22}O$	1-decanol	377.0	374.9	2.1
$C_{11}H_{24}O$	undecanol	419.7	406.7	13.0
$C_{12}H_{26}O$	dodecanol	461.9	438.9	23.0
$C_{13}H_{28}O$	tridecanol	476.1	470.7	5.4
$C_{14}H_{30}O$	1-tetradecanol	505.8	502.5	3.3
$C_{15}H_{28}O$	3,7,11-trimethyl-1-dodecen-3-ol	574.5	496.2	78.3
$C_{15}H_{32}O$	1-pentadecanol	535.1	534.3	0.8
$C_{16}H_{34}O$	1-hexadecanol	523.8	566.1	-42.3
$C_{18}H_{34}O_3$	12-hydroxyoleic acid	646.0	667.8	-21.8
$C_{20}H_{38}O$	3,7,11,15-tetramethyl-1-hexadecyn-3-ol	712.5	659.0	53.5
$C_{20}H_{40}O$	3,7,11,15-tetramethyl-1-hexadecen-3-ol	729.7	649.4	80.3

Liquid Phenols

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_6H_6O	phenol	200.0	177.4	22.6
C_7H_8O	o-hydroxytoluene	233.5	205.9	27.6
C_7H_8O	p-hydroxytoluene	220.9	205.9	15.0
C_7H_8O	m-hydroxytoluene	225.1	205.9	19.2
$C_9H_{12}O$	2,4,6-trimethylphenol	224.7	262.8	-38.1
$C_9H_{12}O_2$	trimethylhydroquinone	217.6	309.2	-91.6

$C_{10}H_8O$	α-napthol	284.5	251.9	32.6

Liquid Carboxylic Acids

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
CH_2O_2	methanoic acid	99.2	87.4	11.8
$C_2H_4O_2$	ethanoic acid	123.0	122.2	0.8
$C_3H_6O_2$	propionic acid	152.7	154.4	-1.7
$C_4H_6O_2$	methacrylic acid	161.1	169.9	-8.8
$C_4H_8O_2$	butanoic acid	177.8	186.2	-8.4
$C_5H_{10}O_2$	pentanoic acid	210.5	218.0	-7.5
$C_5H_{10}O_2$	3-methylbutanoic acid	197.1	211.3	-14.2
$C_6H_{12}O_2$	hexanoic acid	223.8	249.8	-26.0
$C_8H_{16}O_2$	octanoic acid	304.6	313.8	-9.2
$C_9H_{18}O_2$	nonanoic acid	362.3	345.6	16.7
$C_{16}H_{32}O_2$	hexadecanoic acid	677.3	568.6	109.2

Parameters derived from the correlation:	Group	Entries
hydroxyl group (l):	53.1	73
carboxylic acid (l):	87.4	13

Liquid Chlorides

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
CCl_4	carbon tetrachloride	131.8	137.2	-5.4
$CHCl_3$	chloroform	114.2	115.1	-0.9
CH_2Cl_2	dichloromethane	100.0	93.7	6.3
CH_3Cl	methyl chloride	80.8	65.7	15.1
C_2Cl_4	tetrachloroethene	157.7	166.5	-8.8
C_2HCl_3	trichloroethylene	124.7	141.8	-17.1
C_2HCl_5	pentachloroethane	196.2	190.8	5.4
$C_2H_2Cl_2$	1,1-dichloroethene	111.3	109.2	2.1
$C_2H_2Cl_2$	*cis* dichloroethene	113.8	117.2	-3.4
$C_2H_2Cl_2$	*trans* dichloroethene	113.0	117.2	-4.2
$C_2H_2Cl_2O_2$	dichloroacetic acid	188.3	171.5	16.8
$C_2H_2Cl_4$	1,1,2,2-tetrachloroethane	165.3	168.2	-2.9
C_2H_3Cl	vinyl chloride	89.5	84.5	5.0
$C_2H_3ClO_2$	chloroacetic acid	179.9	150.2	29.7
$C_2H_3Cl_3$	1,1,1-trichloroethane	144.3	141.4	2.9
$C_2H_4Cl_2$	1,2-dichloroethane	128.9	125.5	3.4
$C_2H_4Cl_2$	1,1-dichloroethane	126.4	118.8	7.6
C_2H_5Cl	chloroethane	109.2	97.5	11.7
$C_3H_4Cl_4$	1,1,1,3-tetrachloropropan	196.2	201.3	-5.1
C_3H_5Cl	3-chloropropene	125.1	116.3	8.8
$C_3H_5Cl_3$	1,2,3-trichloropropane	172.8	178.7	-5.9
$C_3H_6Cl_2$	2,2-dichloropropane	151.0	145.2	5.8
$C_3H_6Cl_2$	1,2-dichloropropane	154.4	151.0	3.4

C_3H_7Cl	1-chloropropane	130.5	129.3	1.2
$C_4H_8Cl_2$	1,4-dichlorobutane	183.7	189.1	-5.4
C_4H_9Cl	isobutyl chloride	158.6	154.8	3.8
C_4H_9Cl	t-butyl chloride	172.8	149.4	23.4
$C_5H_{11}Cl$	isoamyl chloride	179.5	186.6	-7.1
$C_6H_3Cl_3$	1,2,4-trichlorobenzene	195.0	203.8	-8.8
$C_6H_4Cl_2$	1,2-dichlorobenzene	171.1	179.5	-8.4
$C_6H_4Cl_2$	1,3-dichlorobenzene	171.1	179.5	-8.4
C_6H_5Cl	chlorobenzene	154.0	155.2	-1.2
$C_6H_{12}Cl_2$	1,6-dichlorohexane	239.7	253.1	-13.4
C_7H_7Cl	benzyl chloride	182.4	187.0	-4.6
$C_{10}H_7Cl$	1-chloronaphthalene	211.3	229.3	-18.0
$C_{13}H_{11}Cl$	diphenylchloromethane	290.4	302.1	-11.7
$C_{18}H_{37}Cl$	1-chlorooctadecane	606.7	607.5	-0.8

Parameter derived from the correlation:	Group	Entries
chlorine (1):	30.8	37

Liquid Bromides

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
CBr_4	carbon tetrabromide	162.3	152.3	10.0
$CBrCl_3$	bromotrichloromethane	148.5	141.0	7.5
$CHBr_3$	bromoform	135.1	126.4	8.7
CH_2Br_2	dibromomethane	105.4	101.3	4.1
CH_3Br	bromomethane	78.7	69.5	9.2
$C_2H_2Br_4$	1,1,2,2-tetrabromoethane	154.4	183.3	-28.9
C_2H_3Br	vinyl bromide	107.5	88.3	19.2
$C_2H_4Br_2$	1,2-dibromoethane	136.0	133.1	2.9
C_2H_4BrCl	1-bromo-2-chloroethane	130.1	129.3	0.8
$C_3H_5Br_3$	1,2,3-tribromopropane	166.5	190.0	-23.5
$C_3H_6Br_2$	1,3-dibromopropane	159.0	164.8	-5.8
$C_3H_6Br_2$	1,2-dibromopropane	172.8	158.6	14.2
C_3H_7Br	1-bromopropane	130.5	133.1	-2.6
C_3H_7Br	2-bromopropane	132.2	126.8	5.4
C_4H_9Br	1-bromobutane	152.3	165.3	-13.0
C_4H_9Br	*tert*-butyl bromide	151.0	153.1	-2.1
C_4H_9Br	isobutyl bromide	158.6	158.6	0.0
$C_5H_{11}Br$	1-bromopentane	174.9	197.1	-22.2
$C_5H_{11}Br$	isoamyl bromide	187.0	190.4	-3.4
C_6H_4BrCl	2-bromochlorobenzene	177.0	183.3	-6.3
C_6H_4BrCl	3-bromochlorobenzene	182.0	183.3	-1.3
$C_6H_4Br_2$	1,2-dibromobenzene	196.6	187.0	9.6
$C_6H_4Br_2$	1,3-dibromobenzene	192.0	187.0	5.0
$C_6H_4Br_2O$	2,4-dibromophenol	259.4	233.9	25.5
C_6H_5Br	bromobenzene	154.0	159.0	-5.0
$C_6H_{13}Br$	1-bromohexane	203.8	228.9	-25.1

Parameter derived from the correlation:	Group	Entries
bromine (1):	34.6	26

Liquid Iodides

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
CH_3I	methyl iodide	82.8	74.1	8.7
C_2H_5I	iodoethane	115.1	105.9	9.2
C_3H_7I	iodopropane	126.8	137.7	-10.9
C_4H_9I	isobutyl iodide	162.3	163.2	-0.9
$C_5H_{11}I$	isoamyl iodide	178.7	195.0	-16.3
C_6H_4BrI	2-bromoiodobenzene	179.9	191.6	-11.7
C_6H_4BrI	3-bromoiodobenzene	183.3	191.6	-8.3
C_6H_5I	iodobenzene	158.6	163.6	-5.0

Parameter derived from the correlation:	Group	Entries
iodine (l):	39.1	8

Liquid Esters

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
$C_2H_4O_2$	methyl formate	119.7	97.9	21.8
$C_3H_8O_2$	methyl acetate	112.5	133.1	-20.6
$C_3H_8O_2$	ethyl formate	144.3	130.1	14.2
$C_4H_5ClO_2$	ethyl trichloroacetate	230.1	236.4	-6.3
$C_4H_6Cl_2O_2$	ethyl dichloroacetate	209.6	214.2	-4.6
$C_4H_6O_2$	vinyl acetate	169.5	151.5	18.0
$C_4H_6O_2$	methyl propenoate	159.0	151.5	7.5
$C_4H_8O_2$	ethyl acetate	169.0	164.8	4.2
$C_4H_8O_2$	methyl propionate	172.8	164.8	8.0
$C_4H_8O_2$	propyl formate	171.5	161.9	9.6
$C_5H_8O_2$	allyl acetate	184.1	183.7	0.4
$C_5H_8Cl_2O_2$	ethyl 2,3-dichloropropana	248.9	246.0	2.9
$C_5H_8O_2$	methyl 2-methylpropenoate	188.7	180.3	8.4
$C_5H_9ClO_2$	ethyl 2-chloropropanate	220.5	218.0	2.5
$C_5H_{10}O_2$	isopropyl acetate	196.6	190.4	6.2
$C_5H_{10}O_2$	propyl acetate	194.1	196.6	-2.5
$C_5H_{10}O_2$	methyl butanoate	200.8	196.6	4.2
$C_5H_{10}O_2$	isobutyl formate	214.2	187.0	27.2
$C_5H_{10}O_2$	ethyl propanoate	199.6	196.6	3.0
$C_5H_{10}O_2$	n-butyl methanoate	200.4	196.6	3.8
$C_6H_8O_2$	methyl cyclobutanecarboxy	190.8	196.2	-5.4
$C_6H_8O_2$	ethyl cyclopropanecarboxy	213.0	202.1	10.9
$C_6H_8O_2$	methyl bicyclobutane-1-carboxylate	192.9	188.3	4.6
$C_6H_8O_4$	dimethyl maleate	263.2	251.5	11.7
$C_6H_{10}O_4$	ethylene glycol diacetate	269.0	259.8	9.2
$C_6H_{10}O_4$	diethyl oxalate	260.7	259.8	0.9
$C_6H_{12}O_2$	t-butyl acetate	231.0	216.7	14.3
$C_6H_{12}O_2$	methyl pivalate	223.0	216.7	6.3
$C_6H_{12}O_2$	isobutyl acetate	240.2	222.2	18.0
$C_6H_{12}O_2$	ethyl butanoate	220.1	228.4	-8.3

$C_6H_{12}O_2$	n-butyl acetate	225.1	228.4	-3.3
$C_6H_{12}O_2$	n-propyl propanoate	226.8	228.4	-1.6
$C_7H_{14}O_2$	ethyl pentanoate	229.3	260.2	-30.9
$C_7H_{14}O_2$	ethyl 2,2-dimethylpropionate	251.5	248.5	3.0
$C_7H_{14}O_2$	pentyl ethanoate	276.1	260.2	15.9
$C_7H_{14}O_3$	2-hydroxyethyl 2',2'-dimethylpropionate	307.9	298.7	9.2
$C_8H_8O_2$	methyl benzoate	216.3	222.2	-5.9
$C_8H_8O_3$	methyl o-hydroxybenzoate	268.6	264.8	3.8
$C_8H_{14}O_2$	butyl methacrylate	273.6	276.1	-2.5
$C_8H_{14}O_4$	ethylene glycol dipropanoate	331.8	323.4	8.4
$C_8H_{14}O_4$	diethyl succinate	330.5	323.4	7.1
$C_8H_{16}O_2$	isoamyl propionate	285.3	285.8	-0.5
$C_8H_{16}O_2$	butyl butanoate	282.0	292.5	-10.5
$C_8H_{16}O_2$	pentyl propionate	239.3	292.5	-53.2
$C_8H_{16}O_2$	hexyl ethanoate	282.8	292.5	-9.7
$C_8H_{16}O_2$	methyl heptanoate	284.9	292.5	-7.6
$C_9H_{10}O_2$	benzyl acetate	250.2	254.4	-4.2
$C_9H_{10}O_2$	ethyl benzoate	241.8	254.4	-12.6
$C_9H_{14}O_6$	glycerol triacetate	402.1	380.3	21.8
$C_9H_{18}O_2$	pentyl butanoate	311.7	324.3	-12.6
$C_{10}H_{10}O_4$	1,2-dicarbomethoxybenzene	303.8	313.8	-10.0
$C_{10}H_{18}O_4$	ethylene glycol dibutanoate	380.3	391.6	-11.3
$C_{11}H_{12}O_2$	*trans* ethyl cinnamate	274.1	309.6	-35.5
$C_{11}H_{12}O_2$	benzyl methacrylate	269.9	301.7	-31.8
$C_{11}H_{12}O_2$	4-carbomethoxyhomocubane	287.9	286.2	1.7
$C_{11}H_{14}O_2$	ethyl 3-phenylpropanoate	286.6	318.0	-31.4
$C_{11}H_{22}O_2$	methyl decanoate	382.8	387.9	-5.1
$C_{12}H_{14}O_4$	diethyl o-phthalate	366.1	377.8	-11.7
$C_{12}H_{14}O_4$	diethyl terephthalate	380.7	377.8	2.9
$C_{12}H_{20}O_6$	tripropionin	483.3	476.1	7.2
$C_{12}H_{22}O_2$	octyl methacrylate	386.2	403.3	-17.1
$C_{14}H_{26}O_2$	decyl methacrylate	453.1	467.4	-14.3
$C_{15}H_{26}O_6$	glycerol tributyrate	569.0	571.5	-2.5
$C_{15}H_{30}O_2$	methyl tetradecanoate	505.4	515.5	-10.1
$C_{18}H_{34}O_4$	di-n-butyl sebacate	619.2	642.2	-23.0
$C_{21}H_{38}O_6$	glyceryl tricaproate	753.1	762.7	-9.6
$C_{22}H_{42}O_4$	di-n-hexyl sebacate	732.2	769.9	-37.7
$C_{22}H_{42}O_4$	di-(2-ethylhexyl) adipate	701.7	756.9	-55.2
$C_{22}H_{42}O_4$	di-n-hexyl sebacate	710.9	769.9	-59.0
$C_{24}H_{38}O_4$	di-(2-ethylhexyl) o-phthalate	704.6	747.3	-42.7
$C_{25}H_{48}O_4$	*bis*-(2-ethylhexyl)nonadioate	799.6	852.7	-53.1
$C_{26}H_{50}O_4$	di-n-octyl sebacate	849.4	897.5	-48.1
$C_{33}H_{62}O_6$	glyceryl tridecanoate	1108.8	1145.6	-36.8

Parameter derived from the correlation:	Group	Entries
ester (1):	63.2	72

Liquid Ethers

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_2H_6C	dimethyl ether	102.5	99.6	2.9
$C_3H_8O_2$	2,4-dioxapentane	163.6	161.1	2.5
$C_3H_8O_2$	2-methoxyethanol	174.9	181.6	-6.7
C_4H_8O	2-methoxy-1-propene	162.3	112.1	50.2
$C_4H_{10}O$	methyl isopropyl ether	161.9	156.9	5.0
$C_4H_{10}O$	diethyl ether	172.4	163.2	9.2
$C_4H_{10}O$	methyl propyl ether	165.3	163.2	2.1
$C_4H_{10}O_2$	1,2-dimethoxyethane	193.3	192.9	0.4
$C_4H_{10}O_2$	2-ethoxyethanol	210.9	209.2	1.7
$C_4H_{10}O_3$	1,5-dihydroxy-3-oxapentane	244.8	263.6	-18.8
$C_5H_{12}O$	methyl t-butyl ether	187.4	183.3	4.1
$C_5H_{12}O$	methyl butyl ether	192.9	195.0	-2.1
$C_5H_{12}O$	ethyl propyl ether	197.1	195.0	2.1
$C_5H_{12}O_2$	2,5-dioxaheptane	224.7	225.1	-0.4
$C_5H_{12}O_2$	2-n-propoxyethanol	241.4	245.2	-3.8
$C_5H_{12}O_2$	2-isopropoxyethanol	238.9	238.9	0.0
$C_5H_{12}O_2$	2,2-dimethoxypropane	217.6	213.0	4.6
$C_6H_{10}O_2$	3,6-dioxaoctane	261.1	256.9	4.2
$C_6H_{12}O$	isobutyl vinyl ether	231.8	207.5	24.3
$C_6H_{12}O$	n-butyl vinyl ether	231.8	214.2	17.6
$C_6H_{14}O$	t-butyl ethyl ether	217.6	215.1	2.5
$C_6H_{14}O$	t-amyl methyl ether	221.8	215.1	6.7
$C_6H_{14}O$	isopropyl ether	216.3	214.2	2.1
$C_6H_{14}O$	4-oxaheptane	221.8	227.2	-5.4
$C_6H_{14}O_2$	1,2-diethoxyethane	259.4	256.9	2.5
$C_6H_{14}O_2$	1,1-diethoxyethane	237.7	250.2	-12.5
$C_6H_{14}O_2$	2,5-dioxaoctane	248.9	256.9	-8.0
$C_6H_{14}O_2$	2-butoxyethanol	273.2	277.4	-4.2
$C_6H_{14}O_2$	3-oxa-1-heptanol	273.2	277.4	-4.2
$C_6H_{14}O_3$	2,5,8-trioxanonane	279.9	286.6	-6.7
$C_6H_{14}O_4$	1,8-dihydroxy-3,6-dioxaoctane	327.6	357.3	-29.7
C_7H_8O	anisole	199.2	189.1	10.1
$C_7H_{16}O$	4,4-dimethyl-3-oxahexane	242.7	246.9	-4.2
$C_7H_{16}O_2$	2,5-dioxanonane	282.0	288.7	-6.7
$C_8H_{10}O$	ethyl phenyl ether	228.4	220.9	7.5
$C_8H_{10}O_2$	2-phenoxyethanol	294.6	271.1	23.5
$C_8H_{18}O$	di-t-butyl ether	276.1	266.9	9.2
$C_8H_{18}O$	di-n-butyl ether	278.2	290.8	-12.6
$C_8H_{18}O_2$	4,7-dioxadecane	309.2	320.5	-11.3
$C_8H_{18}O_2$	3,6,9-trioxaundecane	347.3	350.2	-2.9
$C_8H_{18}O_3$	2-(2-butoxyethoxy)ethanol	354.8	370.7	-15.9
$C_8H_{18}O_4$	2,5,8,11-tetradodecane	368.2	380.3	-12.1
$C_8H_{18}O_5$	1,11-dihydroxy-3,6,9-trioxaundecane	428.9	450.6	-21.7
$C_9H_{18}O_4$	2-(2'hydroxyethoxy)ethyl pivalate	311.7	392.0	-80.3
$C_9H_{20}O_4$	tripropylene glycol	440.6	433.5	7.1
$C_{10}H_{12}O_2$	eugenol	343.1	314.6	28.5
$C_{10}H_{22}O_2$	6-methyl-5,7-dioxaundecane	352.3	377.8	-25.5

$C_{10}H_{22}O_6$	1,14-dihydroxy-3,6,9,12-tetraoxatetradecane	515.5	544.3	-28.8
$C_{11}H_{24}O$	methyl n-decyl ether	370.7	386.6	-15.9
$C_{12}H_{26}O_5$	tetrapropylene glycol	559.8	552.3	7.5
$C_{12}H_{26}O_7$	hexaethylene glycol	620.1	637.6	-17.5
$C_{15}H_{32}O_6$	pentapropylene glycol	685.8	671.1	14.7
$C_{18}H_{38}O_7$	hexapropylene glycol	807.5	790.4	17.1
$C_{24}H_{32}O_3$	4-n-heptoxyphenyl 4'-n-butylbenzoate	793.3	685.3	108.0

Parameter derived from the correlation:	Group	Entries
ether (1):	29.8	54

Liquid Nitro Compounds

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
CH_3NO_2	nitromethane	105.9	93.3	12.6
$C_2H_5NO_2$	nitroethane	134.3	125.5	8.8
$C_6H_5NO_2$	nitrobenzene	186.6	182.8	3.8
$C_7H_7NO_2$	4-nitrotoluene	172.4	211.3	-38.9
$C_7H_7NO_2$	3-nitrotoluene	202.5	211.3	-8.8
$C_7H_7NO_2$	2-nitrotoluene	202.1	211.3	-9.2

Parameter derived from the correlation:	Group	Entries
nitro group (1):	[58.6]	6

Liquid Primary Amines

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
$C_2H_8N_2$	diaminoethane	172.8	182.4	-9.6
C_3H_7N	cyclopropylamine	147.3	131.8	15.5
C_3H_9N	1-aminopropane	166.5	158.2	8.3
C_3H_9N	2-aminopropane	164.0	151.5	12.5
$C_3H_{10}N_2$	1,2-diaminopropane	205.9	207.9	-2.0
$C_4H_{11}N$	butylamine	187.9	190.0	-2.1
$C_4H_{11}N$	isobutylamine	194.1	183.3	10.8
$C_4H_{11}N$	t-butylamine	192.0	177.8	14.2
$C_4H_{11}NO$	3-methoxypropylamine	225.5	219.7	5.8
$C_4H_{12}N_2$	1,2-diamino-2-methylpropane	234.7	234.3	0.4
$C_5H_{11}N$	cyclopentylamine	181.2	183.7	-2.5
$C_5H_{13}N$	n-pentylamine	218.0	221.8	-3.8
C_6H_6ClN	m-chloroaniline	198.7	207.9	-9.2
C_6H_7N	aniline	178.7	183.7	-5.0
$C_6H_{15}N$	n-hexylamine	251.9	253.6	-1.7
C_7H_9N	benzylamine	207.1	215.5	-8.4
C_7H_9N	2-methylaniline	209.6	212.1	-2.5
C_7H_9N	3-methylaniline	216.7	212.1	4.6
$C_8H_{11}N$	phenylethylamine	239.3	247.7	-8.4
$C_8H_{11}N$	2,6-dimethylaniline	238.9	240.6	-1.7

$C_9H_{13}N$	3-phenylpropylamine	265.7	279.5	-13.8

Parameter derived from the correlation:	Group	Entries
primary sp^3 nitrogen (1):	59.4	21

Liquid Nitriles

Compounds		Heat Capacities J/(K mole) C_p(l) Expt	C_p(l) Calc	Expt-Calc
C_2H_3N	acetonitile	91.6	82.4	9.2
C_3H_3N	acrylonitrile	108.8	101.3	7.5
C_3H_3N	propionitrile	119.7	114.6	5.1
C_3H_7N	2-cyanopropane	156.1	139.7	16.4
C_4H_5N	cyclopropylcyanide	115.5	120.1	-4.6
C_5H_5N	1-cyanobicyclobutane	131.8	138.1	-6.3
C_7H_9N	1-cyanobicyclo[3.1.0]hexane	170.3	190.0	-19.7
C_5H_9N	2-cyano-2-methylpropane	179.5	207.9	-28.4
$C_5H_6N_2$	1,3-dicyanopropane	183.3	191.2	-7.9
C_5H_7N	cyanocyclobutane	146.0	146.0	0.0
$C_5H_7NO_2$	ethyl cyanoacetate	220.1	209.6	10.5
C_6H_7N	1-cyano-3-methylene-cyclobutane	190.8	166.9	23.9
C_6H_7N	1-cyanobicyclo[2.1.0]pentane	164.0	164.0	0.0
C_6H_9N	1-cyanocyclopentane	167.4	172.0	-4.6
$C_6H_{11}NO_2$	1,1-dimethoxy-3-cyanopropane	253.6	263.2	-9.6
C_7H_5N	benzonitrile	165.3	172.0	-6.7
$C_7H_{11}N$	1-cyanocyclohexane	177.8	197.5	-19.7

Parameter derived from the correlation:	Group	Entries
nitrile group (1):	47.7	17

Liquid Isocyanates

Compounds		Heat Capacities J/(K mole) C_p(l) Expt	C_p(l) Calc	Expt-Calc
C_7H_4ClNO	m-chlorophenylisocyanate	187.0	206.7	-19.7
$C_8H_{12}N_2O_2$	1,6-diisocyanatohexane	299.2	307.5	-8.3
$C_{13}H_{15}NO$	1-(1-isocyanato-1-methylethyl)-3-(1-methylethenyl)benzene	382.0	341.8	40.2
$C_{14}H_{16}N_2O_2$	1,3-*bis*-(1-isocyanato-1-methylethyl)benzene	464.0	401.7	62.3
$C_{14}H_{16}N_2O_2$	1,4-*bis*-(1-isocyanato-1-methylethyl)benzene	415.1	401.7	13.4

Parameter derived from the correlation:	Group	Entries
isocyanate group (1):	[58.2]	5

Liquids Containing Cyclic Tertiary sp^2 Nitrogen

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_5H_5N	pyridine	132.6	129.7	2.9
C_6H_7N	2-methylpyridine	158.6	158.2	0.4
C_6H_7N	3-methylpyridine	158.6	158.2	0.4
C_6H_7N	4-methylpyridine	159.0	158.2	0.8
C_7H_9N	2,3-dimethylpyridine	189.5	186.2	3.3
C_7H_9N	2,4-dimethylpyridine	184.9	186.2	-1.3
C_7H_9N	2,5-dimethylpyridine	184.5	186.2	-1.7
C_7H_9N	2,6-dimethylpyridine	185.4	186.2	-0.8
C_7H_9N	3,4-dimethylpyridine	192.0	186.2	5.8
C_7H_9N	3,5-dimethylpyridine	184.5	186.2	-1.7
C_9H_7N	quinoline	199.2	203.8	-4.6
C_9H_7N	isoquinoline	196.2	203.8	-7.6

Parameter derived from the correlation:	Group	Entries
cyclic tertiary sp^2 nitrogen (l):	20.7	12

Liquids Containing Tertiary sp^2 Nitrogen

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
$C_{18}H_{21}NO$	N-(4-methoxybenzylidene)-p-(n-butyl)aniline	489.9	502.9	-13.0
$C_{18}H_{22}N_2O$	4-ethoxy-4'-butylazobenzene	535.1	551.5	-16.4
$C_{20}H_{24}N_2O_3$	4-methyoxy-4'heptanoyl-azobenzene	685.8	646.4	39.4

Parameter derived from the correlation:	Group	Entries
tertiary sp^2 nitrogen (l):	[44.4]	3

Liquids Containing Cyclic Tertiary sp^3 Nitrogen

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_5H_7N	N-methylpyrrole	150.2	142.7	7.5
$C_6H_{13}N$	N-methylpiperidine	184.9	192.9	-8.0
$C_6H_{15}N_3$	N-(2-aminoethyl)piperazine	284.1	301.2	-17.1
$C_8H_{20}N_4$	N,N'-di(2-aminoethyl) piperazine	407.1	407.1	0.0
$C_{10}H_{22}N_4$	dipiperazinylethane	539.7	420.1	119.6
$C_{10}H_{25}N_5$	N-(2-aminoethyl)-N'-[(2-aminoethyl)-2-aminoethyl]piperazine	528.9	505.8	23.1

Parameter derived from the correlation:	Group	Entries
cyclic tertiary sp^3 nitrogen:	[28.6]	6

Liquids Containing Cyclic Secondary sp^3 Nitrogen Groups

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_4H_5N	pyrrole	127.6	133.1	-5.5
C_4H_9N	pyrrolidine	156.5	149.4	7.1
$C_5H_{11}N$	piperidine	179.9	175.3	4.6
$C_5H_{11}N$	3-methylpyrrolidine	188.3	179.1	9.2
C_6H_9N	2,4-dimethylpyrrole	192.0	201.7	-9.7
C_6H_9N	2,5-dimethylpyrrole	195.4	202.1	-6.7
$C_6H_{13}N$	2-methylpiperidine	205.0	205.0	0.0
$C_6H_{13}N$	4-methylpiperidine	209.2	205.0	4.2
$C_7H_{15}N$	octahydroazocine	230.1	227.2	2.9
$C_8H_{20}N_4$	N-[(2-aminoethyl)-2-aminoethyl]piperazine	391.2	415.9	-24.7
$C_9H_{11}N$	1,2,3,4-tetrahydroquinoline	217.1	241.4	-24.3

Parameter derived from the correlation:	Group	Entries
cyclic secondary sp^3 nitrogen (l):	46.0	11

Liquid Secondary Amines

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_2H_7N	dimethyl amine	136.8	120.9	15.9
$C_2H_8N_2$	N,N'-dimethylhydrazine	171.1	172.0	-0.9
$C_5H_{14}N_2$	N,N-dimethyl-1,3-propanediamine	255.6	267.4	-11.8
$C_6H_8N_2$	phenylhydrazine	217.1	234.7	-17.6
$C_6H_{15}N$	dipropylamine	252.7	248.1	4.6
C_7H_9N	N-methylaniline	207.1	210.0	-2.9

Parameter derived from the correlation:	Group	Entries
secondary sp^3 nitrogen (l):	[51.0]	6

Liquid Secondary Amides

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_2H_5NO	N-methylformamide	123.8	115.1	8.7
C_4H_9NO	N-methylpropanamide	179.1	181.6	-2.5
C_4H_9NO	N-ethylacetamide	179.9	181.6	-1.7
$C_5H_{11}NO$	N-isopropylacetamide	210.9	207.1	3.8
$C_5H_{11}NO$	2,N-dimethylpropanamide	209.2	207.1	2.1
$C_5H_{11}NO$	N-propylacetamide	207.1	213.4	-6.3
$C_5H_{11}NO$	N-methylbutanamide	207.1	213.4	-6.3

$C_6H_{13}NO$	N-n-butylacetamide	236.0	245.2	-9.2
$C_6H_{13}NO$	N-methylpentanamide	238.5	245.2	-6.7

Parameter derived from the correlation:	Group	Entries
secondary amide (1):	79.9	9

Liquid Tertiary sp^3 Nitrogen

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
$C_2H_8N_2$	N,N-dimethylhydrazine	164.0	151.0	13.0
C_3H_9N	trimethylamine	132.6	126.8	5.8
$C_3H_{10}N_2$	trimethylhydrazine	185.8	177.8	8.0
$C_6H_{15}N$	triethylamine	177.0	222.2	-45.2
$C_6H_{15}NO_3$	triethanolamine	389.1	372.8	16.3
$C_8H_{11}N$	N,N-dimethylaniline	213.4	215.9	-2.5
$C_9H_{13}N$	2,N,N-trimethylaniline	280.3	244.3	36.0
$C_{10}H_{15}N$	N,N-diethylaniline	274.5	279.9	-5.4
$C_{13}H_{13}N$	methyldiphenylamine	301.2	305.4	-4.2
$C_{16}H_{35}N$	N,N-dimethyl-2-pentyl-nonylamine	538.1	534.7	3.4

Parameter derived from the correlation:	Group	Entries
tertiary sp^3 nitrogen (1):	22.0	10

Liquid Cyclic Ethers

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_2H_4O	ethylene oxide	87.0	76.1	10.9
C_3H_6O	propylene oxide	120.5	105.9	14.6
C_3H_6O	oxetane	99.6	102.1	-2.5
$C_3H_6O_2$	1,3-dioxolane	118.0	126.8	-8.8
C_4H_4O	furan	114.6	111.7	2.9
C_4H_8O	tetrahydrofuran	123.8	128.0	-4.2
$C_4H_8O_2$	1,3-dioxane	143.9	152.7	-8.8
$C_4H_8O_2$	1,4-dioxane	153.1	152.7	0.4
C_4H_9NO	morpholine	174.1	174.1	0.0
$C_5H_6Cl_2O$	3,3-bis-(chloromethyl)-oxacyclobutane	218.8	219.7	-0.9
C_5H_6O	2-methylfuran	143.9	111.3	32.6
$C_5H_6O_2$	furfuryl alcohol	215.5	196.2	19.3
$C_5H_{10}O$	tetrahydropyran	140.6	154.0	-13.4
$C_5H_{10}O_2$	1,3-dioxepane	167.4	178.2	-10.8
$C_6H_{10}O$	cyclohexene oxide	166.1	169.5	-3.4
$C_6H_{12}O_3$	2,4,6-trimethyl-1,3,5-trioxane	257.3	240.2	17.1
C_8H_6O	2,3-benzofuran	178.7	186.2	-7.5
C_8H_8O	4,5-dihydro-2,3-benzofuran	188.7	194.1	-5.4

$C_8H_{14}O$	3-oxabicyclo[3.2.2]nonane	184.9	220.9	-36.0
$C_9H_{10}O_2$	phenyl glycidyl ether	276.1	256.9	19.2

Parameter derived from the correlation:	Group	Entries
cyclic ethers (1):	24.6	20

Liquid Lactones

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
$C_4H_6O_2$	butyrolactone	141.4	144.8	-3.4
$C_5H_8O_2$	δ-valerolactone	171.5	170.7	0.8
$C_6H_{10}O_2$	ε-caprolactone	196.6	196.6	0.0
$C_{11}H_{20}O_2$	undecanolactone	342.7	325.9	16.8

Parameter derived from the correlation:	Group	Entries
lactones (1):	[67.4]	4

Liquid Cyclic Carbonates

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
$C_3H_4O_3$	ethylene carbonate	133.9	143.9	-10.0
$C_4H_5ClO_3$	4-chloro-1,3-dioxolan-2-one	238.1	201.3	36.8
$C_4H_6O_3$	propylene carbonate	167.4	173.2	-5.8
$C_5H_7ClO_3$	4-chloromethyl-1,3-dioxolan-2-one	248.1	220.5	27.6
$C_5H_{10}O_3$	4-methyl-1,3-dioxolan-2-one	174.9	192.5	-17.6

Parameter derived from the correlation:	Group	Entries
cyclic carbonates (1):	[92.0]	5

Liquid Aldehydes

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_2H_4O	ethanal	89.1	92.5	-3.4
C_3H_6O	propanal	134.7	124.7	10.0
$C_4H_5Cl_3O$	2,2,3-trichlorobutanal	241.8	221.3	20.5
C_4H_5NO	β-cyanopropionaldehyde	195.8	170.3	25.5
C_4H_5NO	α-cyanopropionaldehyde	169.5	164.0	5.5
C_4H_6O	2-butenal	148.5	148.1	0.4
C_4H_8O	butanal	163.6	156.5	7.1
$C_5H_4O_2$	furfural	162.8	169.0	-6.2
$C_5H_{10}O$	2,2-dimethylpropanal	192.9	176.1	16.8
$C_5H_{10}O$	pentanal	190.4	188.3	2.1
C_7H_6O	benzaldehyde	172.0	182.0	-10.0
C_4H_5ClO	2,3,3-trichlorobutanal	241.8	221.3	20.5
$C_7H_{14}O$	3-methylhexanal	246.0	245.6	0.4

$C_7H_{14}O$	3,4-dimethylpentanal	235.6	238.9	-3.3
$C_7H_{14}O$	heptanal	230.1	251.9	-21.8
$C_8H_{16}O$	octanal	259.4	284.1	-24.7
$C_9H_{18}O$	nonanal	290.4	315.9	-25.5
$C_{10}H_{16}O$	citral	304.6	325.1	-20.5
$C_{10}H_{20}O$	decanal	319.7	347.7	-28.0

Parameter derived from the correlation:	Group	Entries
aldehyde (1):	57.7	19

Liquids Ketones

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_3H_6O	acetone	124.7	121.3	3.4
C_4H_8O	2-butanone	159.0	153.1	5.9
$C_5H_8O_2$	acetylacetone (enol)	208.4	223.8	-15.4
$C_5H_{10}O$	2-pentanone	184.5	184.9	-0.4
$C_5H_{10}O$	3-methyl-2-butanone	179.9	178.7	1.2
$C_5H_{10}O$	3-pentanone	190.8	184.9	5.9
$C_6H_{10}O$	4-methylpenten-3-oneD	187.9	197.1	-9.2
$C_6H_{10}O_3$	ethyl acetoacetate	246.9	248.1	-1.2
$C_6H_{12}O$	3,3-dimethyl-2-butanone	207.1	205.0	2.1
$C_6H_{12}O$	4-methyl-2-pentanone	211.7	210.5	1.2
$C_6H_{12}O$	2-hexanone	213.4	216.7	-3.3
$C_6H_{12}O$	3-hexanone	216.7	216.7	0.0
$C_7H_{14}O$	diisopropyl ketone	233.9	235.6	-1.7
C_8H_8O	acetophenone	227.6	210.5	17.1
$C_8H_{16}O$	2-octanone	273.2	280.7	-7.5
$C_8H_{14}O$	6-methyl-5-hepten-2-one	268.6	269.4	-0.8
$C_9H_{18}O$	diisobutylketone	297.5	299.6	-2.1
$C_9H_{18}O$	5-nonanone	303.8	312.5	-8.7
$C_{11}H_{22}O$	6-undecanone	362.8	376.1	-13.3
$C_{13}H_{20}O$	6,10-dimethyl-3,5,9-undecatrien-2-one	413.4	409.2	4.2
$C_{13}H_{26}O$	6,10-dimethyl-2-undecanone	428.4	427.2	1.2
$C_{18}H_{32}O$	6,10,14-trimethyl-3,5-pentadecadien-2-one	555.2	566.9	-11.7
$C_{18}H_{36}O$	6,10,14-trimethyl-2-pentadecanone	593.3	579.9	13.4

Parameter derived from the correlation:	Group	Entries
ketone (1):	51.5	23

Liquid Cyclic Ketones

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
$C_6H_{10}O$	cyclohexanone	177.4	175.7	1.7
$C_9H_{14}O$	2,4,6-trimethyl-2-cyclohexen-1-one	258.6	261.1	-2.5

$C_{10}H_{16}O$	pulegone	274.9	292.0	-17.1

Parameter derived from the correlation:	Group	Entries
cyclic ketone (l):	[46.4]	3

Liquid Sulfides

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_2H_6S	dimethyl sulfide	118.0	110.0	8.0
C_3H_8S	ethyl methyl sulfide	144.8	141.8	3.0
$C_4H_{10}S$	diethyl sulfide	171.5	173.6	-2.1
$C_4H_{10}S$	isopropyl methyl sulfide	172.4	167.4	5.0
$C_4H_{10}S$	propyl methyl sulfide	171.5	173.6	-2.1
$C_5H_{12}S$	methyl t-butyl sulfide	200.0	193.7	6.3
$C_5H_{12}S$	butyl methyl sulfide	200.8	205.9	-5.1
$C_5H_{12}S$	ethyl propyl sulfide	198.3	205.9	-7.6
$C_6H_{12}S$	cyclopentyl methyl sulfide	192.9	199.2	-6.3
$C_6H_{14}S$	diisopropyl sulfide	232.2	224.7	7.5
$C_6H_{14}S$	dipropyl sulfide	225.5	237.7	-12.2
C_7H_8S	methylphenylsulfide	205.9	199.6	6.3
$C_8H_{18}S$	di n-butyl sulfide	284.5	301.2	-16.7
$C_{12}H_{10}S$	diphenylsulfide	271.1	289.1	-18.0

Parameter derived from the correlation:	Group	Entries
sulfide (l):	40.3	14

Liquid Disulfides

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
$C_2H_6S_2$	dimethyldisulfide	146.0	144.3	1.7
$C_4H_{10}S_2$	diethyldisulfide	204.2	207.9	-3.7

Parameter derived from the correlation:	Group	Entries
disulfides (l):	[74.5]	2

Liquid Cyclic Sulfides

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_3H_3NS	thiazole	120.9	119.7	1.2
C_3H_6S	thiacyclobutane	112.5	111.3	1.2
C_4H_4S	thiophene	123.8	120.9	2.9
C_4H_5NS	2-methylthiazole	150.6	154.0	-3.4
C_4H_8S	thiacyclopentane	140.2	137.2	3.0
C_5H_6S	2-methylthiophene	149.8	155.2	-5.4
$C_5H_{10}S$	2-methylcyclothiapentane	172.0	166.9	5.1
$C_5H_{10}S$	3-methylcyclothiapentane	172.0	166.9	5.1

$C_5H_{10}S$	thiacyclohexane	163.2	163.2	0.0
C_6H_8S	2,5-dimethylthiophene	178.2	189.5	-11.3
C_7H_5NS	benzothiazole	189.5	194.1	-4.6

Parameter derived from the correlation:	Group	Entries
cyclic sulfides (1):	33.8	11

Liquid Thiols

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
CH_4S	methanethiol	89.1	83.7	5.4
C_2H_6S	ethyl mercaptan	118.0	115.9	2.1
C_3H_8S	1-propanethiol	144.8	147.7	-2.9
C_3H_8S	2-propanethiol	145.2	141.0	4.2
$C_4H_{10}S$	isobutyl mercaptan	172.0	172.8	-0.8
$C_4H_{10}S$	n-butyl mercaptan	172.4	179.5	-7.1
$C_4H_{10}S$	t-butyl mercaptan	174.9	167.4	7.5
$C_4H_{10}S$	2-butanethiol	171.1	172.8	-1.7
$C_5H_{10}S$	cyclopentanethiol	165.3	173.2	-7.9
$C_5H_{12}S$	3-methyl-1-butanethiol	198.3	205.0	-6.7
$C_5H_{12}S$	1-pentanethiol	200.4	211.3	-10.9
$C_5H_{12}S$	2-methyl-2-butanethiol	198.3	199.6	-1.3
C_6H_6S	thiophenol	173.2	173.2	0.0
$C_6H_{12}S$	cyclohexanethiol	192.5	198.7	-6.2
$C_6H_{14}S$	1-hexanethiol	238.1	243.1	-5.0
$C_7H_{16}S$	1-heptanethiol	259.4	275.3	-15.9
$C_8H_{16}S$	1-octanethiol	300.4	307.1	-6.7
$C_{10}H_{22}S$	1-decanethiol	365.3	370.7	-5.4
$C_{12}H_{28}S$	1-dodecanethiol	442.7	434.7	8.0
$C_{14}H_{30}S$	1-tetradecanethiol	501.7	498.3	3.4
$C_{16}H_{34}S$	1-hexadecanethiol	574.0	561.9	12.1
$C_{18}H_{38}S$	1-octadecanethiol	648.5	625.9	22.6
$C_{20}H_{42}S$	eicosanethiol	725.9	689.5	36.4

Parameter derived from the correlation:	Group	Entries
thiols (1):	49.0	23

Liquid Fluorides

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
$CBrF_3$	bromotrifluoromethane	163.6	97.5	66.1
CCl_2F_2	dichlorodifluoromethane	126.8	107.9	18.9
CCl_3F	fluorotrichloromethane	121.8	122.6	-0.8
CF_4	carbon tetrafluoride	79.9	79.1	0.8
$CHClF_2$	chlorodifluoromethane	114.2	85.8	28.4
$CHCl_2F$	dichlorofluoromethane	123.8	100.4	23.4
CHF_3	trifluoromethane	86.6	71.1	15.5
CH_3F_3	1,1,1-trifluoroethane	109.6	97.5	12.1
$C_2Br_2F_4$	dibromotetrafluoroethane	173.6	161.9	11.7

C_2ClF_3	chlorotrifluoroethene	122.6	123.0	-0.4
C_2ClF_5	pentafluorochloroethane	114.2	140.2	-26.0
$C_2Cl_2F_4$	1,2-dichloro-1,1,2,2-tetrafluoroethane	164.0	154.4	9.6
$C_2Cl_4F_2$	tetrachlorodifluoroethane	178.7	183.7	-5.0
$C_2Cl_3F_3$	1,1,1-trichloro-trifluoroethane	168.6	169.0	-0.4
$C_2Cl_3F_3$	1,1,2-trichloro-1,2,2-trifluoroethane	172.8	169.0	3.8
C_2F_3N	trifluoroacetonitrile	118.0	110.5	7.5
C_2F_4	tetrafluoroethylene	113.0	108.4	4.6
C_2F_6	hexafluoroethane	131.4	125.5	5.9
$C_2HBrClF_3$	1-bromo-2-chloro-1,1,2-trifluoroethane	160.2	150.6	9.6
$C_2HBrClF_3$	2-bromo-2-chloro-1,1,1-trifluoroethane	156.5	150.6	5.9
$C_2H_3ClF_2$	1,1-difluoro-1-chloroethane	130.5	112.1	18.4
$C_2H_4F_2$	1,1-difluoroethane	118.4	90.0	28.4
C_3F_6O	hexafluoroacetone	181.2	177.0	4.2
C_3F_8	octafluoropropane	181.6	172.0	9.6
$C_3H_2ClF_5$	3-chloro-1,1,1,3,3-pentafluoropropane	196.6	172.0	24.6
$C_3H_2Cl_3F_3$	1,1,1-trichloro-3,3,3-trifluoropropane	172.8	201.3	-28.5
$C_3H_4ClF_3$	1,1,1-trifluoro-3-chloropropane	171.1	157.3	13.8
$C_4Br_2Cl_2F_6$	1,4-dibromo-2,3-dichloro-hexafluorobutane	289.5	284.1	5.4
C_4F_8	octafluorocyclobutane	209.6	201.7	7.9
C_5F_{12}	perfluoropentane	188.3	264.8	-76.5
$C_6Br_2Cl_3F_9$	1,6-dibromo-2,3,5-trichloro-nonafluorohexane	418.8	391.6	27.2
C_6F_6	hexafluorobenzene	221.8	189.1	32.7
C_6F_{14}	perfluorohexane	240.2	311.3	-71.1
$C_6F_{15}N$	perfluorotriethylamine	379.5	349.4	30.1
$C_6H_4F_2$	1,2-difluorobenzene	159.4	150.2	9.2
$C_6H_4F_2$	1,3-difluorobenzene	157.3	150.2	7.1
$C_6H_4F_2$	1,4-difluorobenzene	157.3	150.2	7.1
C_6H_5F	fluorobenzene	146.4	140.6	5.8
C_7H_7F	4-fluorotoluene	171.1	169.0	2.1
C_7F_8	perfluorotoluene	262.3	235.6	26.7
C_7F_{14}	perfluoromethylcyclohexane	353.1	349.4	3.7
C_7F_{16}	perfluoroheptane	419.7	357.7	62.0
$C_7H_4F_3NO_2$	3-trifluoromethyl-1-nitrobenzene	223.8	238.9	-15.1
$C_7H_5F_3O_2$	3-trifluoromethylbenzoic acid	223.4	267.8	-44.4
$C_{10}F_{14}$	perfluorobicyclo[4.4.0]deca-1,6-diene	428.4	420.1	8.3
$C_{10}F_{18}$	*cis* perfluorodecalin	449.8	472.0	-22.2
$C_{10}F_{18}$	*trans* perfluorodecalin	446.9	472.0	-25.1

Parameter derived from the correlation:	Group	Entries
fluorides (1):	16.2	46

Liquid Quaternary Silicon Compounds

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
CH_3Cl_3Si	trichloromethylsilane	163.2	158.2	5.0
$C_2H_6Cl_2Si$	dichlorodimethylsilane	171.5	162.3	9.2
$(C_2H_6OSi)_n$	poly(dimethylsiloxane	118.0	130.5	-12.5
$C_3H_6Cl_2Si$	dichloromethylvinylsilane	177.8	181.2	-3.4
C_3H_9ClSi	chlorotrimethylsilane	187.4	166.1	21.3
$(C_4H_{10}OSi)_n$	poly(diethylsiloxane)	165.7	194.1	-28.4
$C_4H_{12}O_4Si$	tetramethylsilicate	318.8	289.5	29.3
$C_5H_{12}Si$	vinyltrimethylsilane	198.3	189.1	9.2
$C_5H_{12}Si$	1,1-dimethyl-1-sila-cyclobutane	197.5	178.2	19.3
$C_6H_{18}Si_2$	hexamethyldisilane	256.1	270.7	-14.6
$C_6H_{21}N_3Si_3$	hexamethyltrisilazane	428.0	439.7	-11.7
$C_7H_{17}NSi$	N-(β-trimethylsilylethyl)-ethylenimine	300.8	279.5	21.3
$(C_7H_{17}NSi)_n$	poly-N-(β-trimethylsilyl)-ethylenimine	287.4	284.9	2.5
$(C_8H_{19}NSi)_n$	poly-N-(β-trimethylsilyl-ethyl)azetidine	318.0	316.7	1.3
$C_8H_{19}NSi$	N-(β-trimethylsilylethyl)-trimethylenimine	304.6	305.4	-0.8
$C_8H_{24}Si_4O_4$	octamethyltetrasiloxane	509.6	500.4	9.2
$C_{10}H_{14}Si$	vinyldimethylphenylsilane	284.9	278.7	6.2
$C_{10}H_{26}O_3Si_3$	1,1,3,3-tetraethyl-5,5-dimethylcyclotrisiloxane	502.9	502.9	0.0
$C_{11}H_{16}Si$	vinyldimethylbenzylsilane	312.1	310.5	1.6
$C_{13}H_{26}O_2Si_3$	1,1,1,3,5,5,5-heptamethyl-3-phenyltrisiloxane	519.7	520.5	-0.8
$C_{12}H_{30}O_3Si_3$	1,1,3,3,5,5-hexaethyl-cyclotrisiloxane	535.1	566.9	-31.8
$C_{16}H_{22}OSi_2$	1,1,3,3-tetramethyl-1,3-diphenyldisiloxane	507.9	479.5	28.4
$C_{16}H_{40}O_4Si_4$	octaethylcyclo tetrasiloxane	746.0	755.6	-9.6
$C_{24}H_{28}O_2Si_3$	1,1,1,5,5,5-hexamethyl-3,3-diphenyltrisiloxane	648.1	610.0	38.1

Parameter derived from the correlation:	Group	Entries
quaternary sp^3 silicon (l):	30.9	24

Liquid Acid Chlorides

Compounds		Heat Capacities J/(K mole) $C_p(l)$ Expt	$C_p(l)$ Calc	Expt-Calc
C_3H_5ClO	propanoyl chloride	147.3	129.7	7.6
C_4H_7ClO	butanoyl chloride	170.7	161.5	9.2
C_4H_7ClO	isobutyroyl chloride	131.8	154.8	-23.0
$C_8H_4Cl_2O_2$	phthalyl dichloride	248.5	243.5	5.0

Parameter derived from the correlation:	Group	Entries
acid chlorides (1):	[62.8]	4

Liquid Quaternary Germanium Compounds

Compounds		Heat Capacities J/(K mole) C_p(c) Expt	C_p(c) Calc	Expt-Calc
$C_4H_{12}Ge$	tetramethylgermane	197.1	187.4	9.7
$C_8H_{12}Ge$	tetraethylgermane	294.6	315.1	-20.5

Parameter estimated from the correlation:	Group	Entries
quaternary germanium (1):	[48.1]	2

Miscellaneous Liquids

Compounds		Heat Capacities J/(K mole) C_p(l) Expt	C_p(l) Calc	Expt-Calc
C_2H_6SO	dimethyl sulfoxide	153.1	153.1	
C_3H_7NO	N,N-dimethylformamide	151.9	152.3	
C_4H_7NO	α-pyrrolidone	169.5	169.5	
$C_4H_{12}Sn$	tetramethyl tin	197.9	197.9	
C_5H_9NO	N-methylpyrrolidine	307.9	307.9	
$C_5H_{11}NO$	2,2-dimethylpropanamide	159.8	159.8	

Parameters derived from the correlation:	Group	Entries
sulfoxides (1):	[83.7]	1
tertiary amides (1):	[82.4]	1
cyclic secondary amide (1):	[92.0]	1
cyclic tertiary amide (1):	[170]	1
primary amide group (1):	[41.0]	1
quaternary tin (1):	[58.6]	1

Functional Group Parameters-Solids

Solid Linear Hydrocarbons

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_{16}H_{34}$	hexadecane	441.8	450.2	-8.4
$C_{18}H_{38}$	octadecane	485.8	504.2	-18.4
$C_{20}H_{42}$	eicosane	479.9	558.1	-78.2
$C_{22}H_{46}$	n-docosane	563.6	616.3	-52.7
$C_{24}H_{50}$	tetracosane	730.9	666.1	64.8
$C_{25}H_{52}$	n-pentacosane	769.0	692.9	76.1
$C_{26}H_{54}$	n-hexacosane	661.1	719.6	-58.5
$C_{27}H_{56}$	heptacosane	828.4	746.8	81.6
$C_{30}H_{62}$	triacontane	808.8	827.6	-18.8
$C_{31}H_{64}$	unatriacontane	912.1	854.4	57.7
$C_{32}H_{66}$	dotriacontane	877.4	881.6	-4.2
$C_{33}H_{68}$	triatriacontane	900.8	908.3	-7.5
$C_{34}H_{70}$	tetratriacontane	887.4	935.1	-47.7
$C_{35}H_{72}$	pentatriacontane	915.9	962.3	-46.4

Parameters derived from the correlation:	Group	Entries
primary sp^3 carbon (c):	36.6	14
secondary sp^3 carbon (c):	26.9	14

Solid Aromatic Hydrocarbons

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
C_6H_6	benzene	97.9	105.0	-7.1
$C_{10}H_8$	naphthalene	168.2	157.3	10.9
$C_{10}H_{14}$	1,2,4,5-tetramethylbenzene	215.1	215.5	-0.4
$C_{11}H_{10}$	2-methylnaphthalene	195.8	184.9	10.9
$C_{11}H_{16}$	pentamethylbenzene	251.0	243.1	7.9
$C_{12}H_8$	biphenyl	197.9	192.5	5.4
$C_{12}H_{12}$	1,8-dimethylnaphthalene	242.7	212.5	30.2
$C_{12}H_{12}$	2,3-dimethylnaphthalene	216.3	212.5	3.8
$C_{12}H_{12}$	2,6-dimethylnaphthalene	204.2	212.5	-8.3
$C_{12}H_{12}$	2,7-dimethylnaphthalene	204.6	212.5	-7.9
$C_{12}H_{18}$	hexamethylbenzene	245.6	270.3	-24.7
$C_{13}H_{12}$	diphenylmethane	223.8	219.2	4.6
$C_{14}H_{10}$	phenanthrane	220.5	209.2	11.3
$C_{14}H_{10}$	anthracene	210.5	209.2	1.3
$C_{14}H_{14}$	1,2-diphenylethane	251.0	246.0	5.0
$C_{15}H_{12}$	4-methylphenanthrene	262.8	236.8	26.0
$C_{16}H_{10}$	1,2-benzacenaphthene	230.1	226.8	3.3
$C_{16}H_{10}$	pyrene	229.7	227.2	2.5
$C_{18}H_{12}$	benzanthrene	273.6	261.5	12.1
$C_{18}H_{12}$	triphenylene	259.4	261.5	-2.1
$C_{18}H_{12}$	naphthacene	236.4	261.5	-25.1

$C_{18}H_{14}$	p-terphenyl	278.7	279.5	-0.8
$C_{18}H_{14}$	o-terphenyl	274.9	279.5	-4.6
$C_{20}H_{12}$	perylene	274.9	279.1	-4.2
$C_{21}H_{16}$	1,2'dinaphthylmethane	314.6	323.4	-8.8
$C_{24}H_{12}$	coronene	313.8	314.6	-0.8
$C_{24}H_{18}$	1,3,5-triphenylbenzene	361.1	366.5	-5.4
$C_{24}H_{18}$	p-quaterphenyl	339.7	366.5	-26.8

Parameters derived from the correlation:	Group	Entries
tertiary aromatic sp^2 carbon (c):	17.5	27
quaternary aromatic sp^2 carbon (c):	8.49	27
internal quaternary aromatic sp^2 carbon (c):	~~[4.44]~~ [9.1]	4

Solid Cyclic and Polycyclic Hydrocarbons

	Compounds	Heat Capacities J/(K mole) C_p(c) Expt	C_p(c) Calc	Expt-Calc
C_7H_{10}	nortricyclene	128.9	120.5	8.4
C_7H_{12}	norbornane	151.0	146.4	4.6
C_8H_{14}	bicyclo[2.2.2]octane	157.7	171.1	-13.4
$C_{10}H_{16}$	adamantane	190.0	194.6	-4.6
$C_{10}H_{16}$	tricyclo[5.2.1.$0^{2,6}$]decane	241.4	194.6	46.8
$C_{10}H_{16}$	tricyclo[3.3.1.$1^{3,7}$]decane	190.0	194.6	-4.6
$C_{11}H_{20}$	bicyclo[3.3.3]undecane	213.4	244.8	-31.4
$C_{13}H_{10}$	fluorene	193.7	198.7	-5.0
$C_{14}H_{12}$	9,10-dihydrophenanthrene	243.5	223.4	20.1
$C_{14}H_{14}$	1,2,3,4-tetrahydroanthracene	246.9	237.7	9.2
$C_{14}H_{18}$	1,2,3,4,5,6,7,8-octahydroanthracene	327.6	265.7	61.9
$C_{14}H_{20}$	diamantane	223.4	241.4	-18.0
$C_{14}H_{24}$	*cis-anti-trans*-perhydrophenanthrene	289.5	292.9	-3.4
$C_{14}H_{24}$	*cis-anti-trans*-perhydrophenanthrene	345.6	292.9	52.7
$C_{14}H_{24}$	*trans-anti-trans*-perhydrophenanthrene	281.2	292.9	-11.7
$C_{16}H_{16}$	2,2-metacyclophane	240.6	272.4	-31.8
$C_{16}H_{16}$	2,2-metaparacyclophane	261.5	272.4	-10.9
$C_{16}H_{16}$	2,2-paracyclophane	252.7	272.4	-19.7
$C_{18}H_{16}$	*anti-trans*-truxane	252.7	270.3	-17.6
$C_{18}H_{16}$	*syn-trans*-truxane	275.3	270.3	5.0
$C_{18}H_{18}$	2,2'-biindanyl	332.6	296.2	36.4
$C_{18}H_{20}$	3,3-paracyclophane	324.3	321.7	2.6
$C_{20}H_{14}$	triptycene	282.8	284.9	-2.1
$C_{22}H_{26}$	1.1'diphenyl-1,1'-bicyclopentyl	375.7	401.2	-25.5
$C_{24}H_{30}$	1,1'diphenyl-1,1'-bicyclohexyl	403.8	450.2	-46.4
$C_{26}H_{34}$	1,1'diphenyl-1,1'-bicyclooctyl*	454.0	548.5	-94.5

Parameters derived from the correlation:	Group	Entries
cyclic secondary sp^3 carbon (c):	24.6	27
cyclic tertiary sp^3 carbon (c):	11.7	20
cyclic quaternary sp^3 carbon (c):	6.11	11

* not used in the correlation

Solid Branched Hydrocarbons

	Compounds	Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
C_8H_{18}	2,2,3,3-tetramethylbutane	232.2	209.6	22.6
$C_{18}H_{18}$	1-methyl-7-isopropyl-phenanthrene	294.6	292.9	1.7
$C_{18}H_{22}$	2,3-dimethyl-2,3-diphenylbutane	320.5	328.9	-8.4
$C_{19}H_{16}$	triphenylmethane	308.8	297.5	11.3
$C_{20}H_{18}$	1,1,2-triphenylethane	319.7	324.3	-4.6
$C_{20}H_{18}$	1,1,1-triphenylethane	316.7	320.1	-3.4
$C_{24}H_{46}$	2,11-dicyclohexyldodecane	557.3	584.5	-27.2
$C_{24}H_{46}$	1,1-dicyclohexyldodecane	562.7	584.5	-21.8
$C_{25}H_{20}$	tetraphenylmethane	368.2	379.5	-11.3
$C_{26}H_{22}$	1,1,1,2-tetraphenylethane	395.4	406.7	-11.3
$C_{26}H_{22}$	1,1,2,2-tetraphenylethane	396.6	402.5	-5.9
$C_{26}H_{38}$	2,3-dimethyl-2,3-*bis*-(4-*tert*-butylphenyl)butane	529.7	520.1	9.6
$C_{28}H_{42}$	3,4-dimethyl-3,4-bis-(4-*tert*-butylphenyl)hexane	587.9	574.0	13.9
$C_{32}H_{26}$	pentaphenylethane	473.6	484.5	-10.9
$C_{32}H_{50}$	2,4,5,7-tetramethyl-4,5-*bis*-(4-*tert*-butylphenyl)octane	684.1	665.3	18.8
$C_{32}H_{50}$	4,5-diethyl-4,5-*bis*-(4-*tert*-butylphenyl)octane	618.4	682.0	-63.6
$C_{38}H_{62}$	5,6-dibutyl-5,6-*bis*-(4-*tert*-butylphenyl)decane	805.4	843.5	-38.1

Parameters derived from the correlation:	Group	Entries
tertiary sp^3 carbon (c):	9.00	11
quaternary sp^3 carbon (c):	-4.98	11

Mixed Functional Groups Used to Evaluate Solid Hydrocarbon Parameters

	Compounds	Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_2H_3N_3$	1,2,4-triazole	78.7	83.7	-5.0
$C_4H_2O_4$	squaric acid	121.8	125.1	-3.3
$C_4H_4O_4$	*cis* butenedioic acid	135.6	149.0	-13.4
$C_4H_4O_4$	*trans* butenedioic acid	141.8	149.0	-7.2
$C_4H_5ClO_2$	*cis* 3-chloro-2-butenoic acid	140.2	146.4	-6.2
$C_4H_5ClO_2$	*trans* 3-chloro-2-butenoic acid	159.8	146.4	13.4
$C_5H_8O_2$	methyl 2-methylpropenoate	165.3	166.5	-1.2
$C_6H_8O_4$	dimethyl fumarate	199.2	196.6	2.6
$C_6Cl_4O_2$	tetrachlorobenzoquinone	193.7	202.1	-8.4
$C_6H_4O_2$	p-quinone	126.4	132.2	-5.8
$C_7H_6N_2$	benzimidazole	128.9	141.0	-12.1
C_8H_7N	indole	192.0	142.7	49.3
C_8H_{12}	bicyclo[2.2.2]octene	156.9	153.6	3.3
$C_9H_7NO_4$	o-nitrocinnamic acid	240.6	238.9	1.7

$C_9H_7NO_4$	m-nitrocinnamic acid	240.2	238.9	1.3
$C_9H_7NO_4$	p-nitrocinnamic acid	238.1	238.9	-0.8
$C_9H_8O_2$	cinnamic acid	197.5	192.0	5.5
$C_{10}H_{10}O_2$	4-carboxypentacyclo[4.3.0.$0^{2,5}$.$0^{3,8}$.$0^{4,7}$] nonane	206.7	165.7	41.0
$C_{10}H_{16}O$	(D) camphor	242.7	241.8	0.9
$C_{10}H_{16}O$	(DL) camphor	271.1	241.8	29.3
$C_{11}H_{10}O_4$	p-methacrylolyoxybenzoic acid	257.7	269.9	-12.2
$C_{11}H_{12}N_2O_2$	L-tryptophane	238.1	242.3	-4.2
$C_{11}H_{14}N_2$	3-dimethylaminomethylindole	283.7	270.7	13.0
$C_{11}H_{17}NO$	1-adamantylcarboxamide	220.5	243.5	-23.0
$C_{12}H_8$	acenaphthylene	166.5	166.9	-0.4
$C_{12}H_{12}O_4$	1,4-dimethyl cubane-dicarboxylate	251.0	236.4	14.6
$C_{12}H_{22}O_{11}$	sucrose	425.5	437.6	-12.1
$C_{13}H_{20}O$	4-(2,6,6-trimethyl-1-cyclo-hexen-1-yl)-3-buten-2-one	382.8	306.7	76.1
$C_{14}H_{14}$	*trans*-1,2-diphenylethylene	235.1	235.1	0.0
$C_{16}H_{36}N_4$	*cis*-(5,12)-7,7,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane	444.8	498.3	-53.5
$C_{19}H_{14}N_2$	1,2-diphenylbenzimidazole	318.8	318.8	0.0
$C_{20}H_{16}$	triphenylethylene	309.2	316.7	-7.5
$C_{26}H_{20}$	tetraphenylethylene	388.7	398.3	-9.6
$C_{20}H_{18}Sn$	triphenyl vinyl tin	486.6	433.5	53.1
$C_{22}H_{26}$	1,1'-diphenyl-1,1'-bicyclopentyl	375.3	401.2	-25.9
$C_{24}H_{30}$	1,1'-diphenyl-1,1'-dicyclohexyl	403.8	450.2	-46.4
$C_{26}H_{34}$	1,1'-diphenyl-1,1'-bicyclooctyl	454.0	527.6	-73.6

Parameters derived from the correlation:	Group	Entries
secondary sp^2 carbon (c):	[46.0]	3
tertiary sp^2 carbon (c):	21.4	13
quaternary sp^2 carbon (c):	[6.86]	6
cyclic quaternary sp^3 carbon (c):	6.11	11
cyclic tertiary sp^2 carbon (c):	[15.9]	7
cyclic quaternary sp^2 carbon (c):	[4.73]	5

Mixed Functional Groups Used to Evaluate Solid Hydrocarbon Parameters

Compounds		Heat Capacities J/(K mole) C_p(c) Expt	C_p(c) Calc	Expt-Calc
C_6H_6	2,4-hexadiyne	31.9	32.3	-0.4
$C_{14}H_{10}$	diphenylacetylene	54.0	53.3	0.7
$C_{16}H_{12}Ge$	diethynyldiphenylgermane	73.4	75.6	-2.2
$C_{16}H_{12}Si$	diethynyldiphenylsilane	91.3	78.8	12.4
$C_{26}H_{20}Sn$	triphenyl phenylethynyl tin	107.0	117.7	-10.8
$C_{32}H_{22}Ge$	1,1-diethynyl-2,3,4,5-tetraphenyl-1-germacyclopentadiene	133.0	126.0	7.0

Parameters derived from the correlation:	Group	Entries
tertiary sp carbon:	[37.1]	3
quaternary sp carbon:	[15.5]	6

Solid Hydrocarbon Polymers

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$(CH_2)_n$	polyethylene branched*	31.8	26.8	5.0
$(CH_2)_n$	polyethylene amorphous*	33.1	31.8	1.3
$(CH_2)_n$	polyethylene c*	24.7	26.8	-2.1
$(C_3H_6)_n$	polypropylene,isotatic,,cryst*	69.0	72.4	-3.4
$(C_4H_6)_n$	*trans*-1,4-polybutadiene*	87.4	96.7	-9.3
$(C_4H_8)_n$	polyisobutylene*	109.6	99.2	10.4
$(C_6H_{10})_n$	ethylene-butadiene copolymer*	149.0	150.6	-1.6
$(C_9H_{10})_n$	poly-(a-methylstyrene)*	149.4	154.8	-5.4

*Not Used in Generating Hydrocarbon Parameters

Solid Alcohols

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$(C_2H_4O)_n$	polyvinyl alcohol	46.0	59.4	-13.4
C_3H6O_3	D-lactic acid	127.6	122.2	5.4
C_4H6O_6	tartaric acid	184.5	170.7	13.8
C_4H10O_3	1,1,1-trihydroxymethylpropane	213.8	147.7	66.1
C_8H8O_3	mandelic acid	199.2	181.6	17.6
$C_{13}H_{12}O$	diphenylcarbinol	233.5	224.7	8.8
$C_{13}H_{28}O$	tridecanol	377.8	383.3	-5.5
$C_{13}H_{28}O$	tri-t-butylmethanol	350.6	333.0	17.6
$C_{14}H_{30}O$	1-tetradecanol	387.9	410.5	-22.6
$C_{15}H_{32}O$	1-pentadecanol	400.0	437.2	-37.2
$C_{16}H_{34}O$	1-hexadecanol	422.2	464.0	-41.8
$C_{19}H_{16}O$	triphenylcarbinol	318.8	307.1	11.7

Solid Phenols

C_6H_6O	phenol	127.6	119.7	7.9
$C_6H_6O_2$	1,2-dihydroxybenzene	144.3	133.9	10.4
$C_6H_6O_2$	1,3-dihydroxybenzene	122.6	133.9	-11.3
$C_6H_6O_2$	1,4-dihydroxybenzene	118.8	133.9	-15.1
C_7H_8O	p-hydroxytoluene	150.2	147.3	2.9
$C_7H_8O_2$	2,5-dihydroxytoluene	174.9	161.5	13.4
$C_7H_6O_2$	o-hydroxybenzoic acid	159.4	163.6	-4.2
$C_7H_6O_2$	m-hydroxybenzoic acid	157.3	163.6	-6.3
$C_7H_6O_2$	p-hydroxybenzoic acid	155.2	163.6	-8.4
$C_8H_{10}O$	4-ethylphenol	207.1	174.1	33.0
$C_{10}H_8O$	α-napthol	166.9	171.5	-4.6
$C_{10}H_8O$	β-napthol	172.8	171.5	1.3
$C_{12}H_{10}O$	o-hydroxybiphenyl	235.1	206.7	28.4
$C_{12}H_{10}O_2$	4,4'-dihydroxybiphenyl	224.3	221.3	3.0
$C_{15}H_{16}O_2$	2,2-bis(4-hydroxyphenyl)-propane	287.9	289.5	-1.6

Solid Sugars

$C_4H_{10}O_4$	erythritol	161.9	165.7	-3.8
$C_5H_{12}O_4$	pentaerythritol	190.4	196.6	-6.2
$C_6H_{14}O_6$	D-sorbitol	241.4	231.0	10.4
$C_6H_{14}O_6$	*meso*-galactitol	238.5	231.0	7.5
$C_6H_{14}O_6$	D-mannitol	238.9	231.0	7.9

Solid Acids

$C_2H_2O_4$	oxalic acid	120.1	105.9	14.2
$(C_4H_6O_2)_n$	polymethacrylic acid	92.0	111.7	-19.7
$C_4H_4O_4$	*cis* butenedioic acid	135.6	149.0	-13.4
$C_4H_4O_4$	*trans* butenedioic acid	141.8	149.0	-7.2
$C_4H_6O_4$	succinic acid	153.1	159.8	-6.7
$C_5H_8O_4$	2-methylsuccinic acid	199.6	178.7	20.9
$C_5H_{10}O2$	2,2-dimethylpropanoic acid	177.8	157.7	20.1
$C_6H_8O_7$	citric acid	226.4	231.4	-5.0
$C_6H_{10}O4$	adipic acid	196.6	213.8	-17.2
$C_7H_6O_2$	benzoic acid	146.9	149.0	-2.1
$C_8H_6O_4$	benzene-1,2-dicarboxylic acid	188.3	193.3	-5.0
$C_8H_6O_4$	benzene-1,3-dicarboxylic acid	201.7	193.3	8.4
$C_8H_6O_4$	benzene-1,4-dicarboxylic acid	199.6	193.3	6.3
$C_8H_8O_2$	o-toluic acid	174.9	176.6	-1.7
$C_8H_8O_2$	m-toluic acid	163.6	176.6	-13.0
$C_8H_8O_2$	p-toluic acid	169.0	176.6	-7.6
$C_9H_8O_2$	cinnamic acid	197.5	192.0	5.5
$C_{10}H_{10}O_2$	4-carboxypentacyclo $[4.3.0.0^{2,5}.0^{3,8}.0^{4,7}]$nonane	207.1	165.7	41.4
$C_{10}H_{20}O_2$	decanoic acid	361.1	305.0	56.1
$C_{11}H_{22}O_2$	undecanoic acid	415.1	332.2	82.9
$C_{12}H_{24}O_2$	dodecanoic acid	404.2	359.0	45.2
$C_{13}H_{26}O_2$	tridecanoic acid	387.4	385.8	1.6
$C_{14}H_{28}O_2$	tetradecanoic acid	432.2	413.0	19.2
$C_{15}H_{30}O_2$	pentadecanoic acid	443.5	439.7	3.8
$C_{16}H_{32}O_2$	hexadecanoic acid	460.7	466.9	-6.2
$C_{17}H_{34}O_2$	heptadecanoic acid	475.7	493.7	-18.0
$C_{18}H_{36}O_2$	octadecanoic acid	561.9	520.5	41.4
$C_{19}H_{30}O_2$	nonadecanoic acid	525.5	547.7	-22.2
$C_{20}H_{40}O_2$	eicosanoic acid	545.2	574.5	-29.3

Parameters derived from the correlation:	Group	Entries
hydroxyl group (c):	23.5	33
carboxyl group (c):	53.1	35

Solid Chlorides

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
C_2Cl_6	hexachloroethane	218.0	161.9	56.1
$(C_2H_3Cl)_n$	polyvinyl chloride	59.4	64.4	-5.0
$C_2H_3Cl_3$	1,1,2-trichloroethane	143.1	121.8	21.3
$C_4H_5ClO_2$	*cis* 3-chloro-2-butenoic acid	140.2	146.4	-6.2

$C_4H_5ClO_2$	*trans* 3-chloro-2-butenoic acid	159.8	146.4	13.4
$C_5H_8Cl_4$	pentaerythrityl tetrachloride	198.3	217.6	-19.3
C_6Cl_6	hexachlorobenzene	201.3	223.0	-21.7
C_6HCl_5	pentachlorophenol	202.1	217.6	-15.5
$C_6H_2Cl_4$	1,2,4,5-tetrachlorobenzene	202.5	183.7	18.8
$C_6H_4Cl_2$	1,4-dichlorobenzene	147.7	144.3	3.4
$C_7H_5ClO_2$	2-chlorobenzoic acid	163.2	168.6	-5.4
$C_7H_5ClO_2$	3-chlorobenzoic acid	163.6	168.6	-5.0
$C_7H_5ClO_2$	4-chlorobenzoic acid	167.4	168.6	-1.2
$C_{11}H_{15}Cl$	pentamethylchlorobenzene	244.8	262.8	-18.0
$C_{12}Cl_{10}$	perchlorobiphenyl	343.9	388.3	-44.4
$C_{12}H_9Cl$	2-chlorobiphenyl	207.9	211.7	-3.8
$C_{12}H_9Cl$	4-chlorobiphenyl	243.9	211.7	32.2
$C_{19}H_{15}Cl$	triphenylchloromethane	311.7	312.1	-0.4

Parameter derived from the correlation:	Group	Entries
chlorides (c):	28.7	18

Solid Bromides

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
CBr_4	carbon tetrabromide	128.9	124.7	4.2
$C_2H_2Br_2O_2$	dibromoacetic acid	124.7	126.8	-2.1
$C_3H_6Br_2$	1,3-dibromopropane	156.1	145.6	10.5
$C_5H_8Br_4$	pentaerythrityl tetrabromide	213.8	232.2	-18.4
$C_6H_3Br_3O$	2,4,6-tribromophenol	172.0	160.2	11.8
$C_6H_4Br_2$	p-dibromobenzene	174.5	151.9	22.6
$C_7H_5BrO_2$	2-bromobenzoic acid	154.0	172.4	-18.4
$C_7H_5BrO_2$	3-bromobenzoic acid	151.5	172.4	-20.9
$C_7H_5BrO_2$	4-bromobenzoic acid	151.5	172.4	-20.9

Parameter derived from the correlation:	Group	Entries
bromides (c):	[32.4]	9

Solid Iodides

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_5H_8I_4$	pentaerythrityl tetraiodide	209.6	214.2	-4.6
$C_6H_4I_2$	1,4-diiodobenzene	160.7	143.1	17.6
C_6H_5I	iodobenzene	112.1	123.8	-11.7

Parameter derived from the correlation:	Group	Entries
Iodides (c):	[27.9]	3

Solid Esters

Compounds		Heat Capacities J/(K mole) C_p(c) Expt	C_p(c) Calc	Expt-Calc
$C_5H_8O_2$	methyl 2-methylpropenoate	165.3	166.5	-1.2
$C_6H_8O_4$	dimethyl fumarate	199.2	196.6	2.6
$(C_6H_{10}O_2)_n$	poly-ε-caprolactone	161.5	174.9	-13.4
$C_{10}H_{10}O_4$	1,4-dicarbomethoxybenzene	276.1	241.0	35.1
$C_{10}H_{12}O_4$	2-monobenzoyl glycerol	236.4	246.4	-10.0
$C_{10}H_{12}O_4$	1-monobenzoyl glycerol	238.9	246.4	-7.5
$C_{11}H_{10}O_4$	p-methacrylolyoxybenzoic acid	257.7	269.9	-12.2
$C_{12}H_{12}O_4$	1,4-dimethyl cubane dicarboxylate	251.0	236.4	14.6
$(C_{13}H_{24}O_2)_n$	polytridecanolactone	329.3	363.6	-34.3
$C_{13}H_{26}O_4$	1-monocaprin	410.0	402.5	7.5
$C_{15}H_{30}O_4$	2-monolaurin	436.4	456.1	-19.7
$C_{15}H_{30}O_4$	1-monolaurin	447.7	456.1	-8.4
$C_{16}H_{12}O_4$	dibenzoylethylene	275.3	315.9	-40.6
$C_{16}H_{14}O_4$	dibenzoylethane	291.2	326.8	-35.6
$C_{16}H_{22}O_4$	dibutyl o-phthalate	477.0	402.5	74.5
$C_{17}H_{34}O_2$	methyl hexadecanoate	474.5	490.8	-16.3
$C_{17}H_{34}O_4$	2-monomyristin	506.3	510.0	-3.7
$C_{19}H_{38}O_4$	1-monopalmitin	566.9	564.0	2.9
$C_{19}H_{38}O_4$	2-monopalmitin	558.6	564.0	-5.4
$C_{21}H_{42}O_4$	2-monostearin	610.4	618.0	-7.6
$C_{21}H_{42}O_4$	1-monostearin	610.4	618.0	-7.6
$C_{24}H_{38}O_4$*	di-octyl o-phthalate	707.1	618.0	89.1
$C_{23}H_{44}O_5$*	1-aceto-3-stearin	938.5	669.9	268.6
$C_{25}H_{46}O_6$	1,2-diaceto-3-stearin	904.2	722.6	181.6
$C_{42}H_{66}O_{12}$	benzene-hexa-n-hexanoate	1294.9	1159.0	135.9
$C_{48}H_{78}O_{12}$*	benzene hexa-n-heptanoate	1500.0	1320.5	179.5
$C_{54}H_{90}O_{12}$	benzene hexa-n-octanoate	2131.3	1478.6	652.7

Parameter derived from the correlation:	Group	Entries
ester (c):	40.3	24

*Not used in the correlation

Solid Ethers

Compounds		Heat Capacities J/(K mole) C_p(c) Expt	C_p(c) Calc	Expt-Calc
$C_7H_7NO_3$	p-nitroanisole	279.9	229.7	50.2
$C_8H_8O_3$	4-methoxybenzoic acid	207.5	226.4	-18.9
$C_8H_9NO_3$	p-nitroethoxybenzene	246.0	256.5	-10.5
$C_{12}H_{10}O$	diphenyl ether	215.9	241.8	-25.9
$C_{22}H_{24}O_6$	di(p-methoxyphenyl)-trans-cyclohexane-1,4-dicarboxylate	478.6	549.4	-70.8

Solid Nitro Groups

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_3H_6N_2O_4$	2,2-dinitropropane	206.3	180.3	26.0
$C_6H_3N_3O_7$	1,3,5-trinitrophenol	239.7	260.7	-21.0
$C_6H_3N_3O_6$	1,3,5-trinitrobenzene	222.6	246.4	-23.8
$C_6H_4N_2O_4$	1,2-dinitrobenzene	195.0	199.2	-4.2
$C_6H_4N_2O_4$	1,3-dinitrobenzene	188.3	199.2	-10.9
$C_6H_4N_2O_4$	1,4-dinitrobenzene	192.0	199.2	-7.2
$C_6H_4ClNO_2$	1,2-chloronitrobenzene	247.7	172.0	75.7
$C_6H_4ClNO_2$	1,4-chloronitrobenzene	182.4	172.0	10.4
$C_6H_5NO_3$	4-nitrophenol	143.9	166.5	-22.6
$C_7H_5NO_4$	2-nitrobenzoic acid	191.6	196.2	-4.6
$C_7H_5NO_4$	3-nitrobenzoic acid	179.9	196.2	-16.3
$C_7H_5NO_4$	4-nitrobenzoic acid	180.3	196.2	-15.9
$C_7H_5N_3O_6$	2,4,5-trinitrotoluene	311.7	273.6	38.1
$C_7H_6N_2O_4$	2,4-dinitrotoluene	255.2	226.8	28.4
$C_9H_7NO_4$	o-nitrocinnamic acid	240.6	238.9	1.7
$C_9H_7NO_4$	m-nitrocinnamic acid	240.2	238.9	1.3
$C_9H_7NO_4$	p-nitrocinnamic acid	238.1	238.9	-0.8
$C_7H_8N_2O_2$	5-nitro-2-aminotoluene	217.1	192.5	24.6
$C_7H_8N_2O_2$	3-nitro-4-aminotoluene	205.4	192.5	12.9
$C_{10}H_6N_2O_4$	1,5-dinitronaphthalene	259.4	251.5	7.9
$C_{10}H_6N_2O_4$	1,8-dinitronaphthalene	254.4	251.5	2.9

Solid Primary Amines

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_2H_5NO_2$	glycine	99.2	101.7	-2.5
$C_3H_7NO_2$	D-alanine	120.9	120.1	0.8
$C_3H_7NO_2$	L-alanine	122.2	120.1	2.1
$C_3H_7NO_2$	DL-alanine	121.8	120.1	1.7
$C_3H_7NO_3$	L-serine	135.6	133.9	1.7
$C_3H_7NO_3$	DL-serine	132.2	133.9	-1.7
$C_4H_7NO_4$	L-aspartic acid	155.2	163.6	-8.4
$C_4H_9NO_2$	DL-2-aminobutanoic acid	146.4	147.3	-0.9
$C_5H_9NO_4$	glutamic acid	174.9	190.4	-15.5
$C_5H_{11}NO_2$	L-2-amino-3-methylbutanoic acid	169.0	165.7	3.3
$C_5H_{11}NO_2$	5-aminopentanoic acid	163.6	182.4	-18.8
$C_5H_{12}N_2O_2$	*dl*-2,5-diaminopentanoic acid	191.2	190.4	0.8
$C_6H_4Br_3N$	2,4,6-tribromoaniline	181.6	187.9	-6.3
$C_6H_6N_2O_2$	2-nitroaniline	168.2	164.8	3.4
$C_6H_6N_2O_2$	3-nitroaniline	159.0	164.8	-5.8
$C_6H_6N_2O_2$	4-nitroaniline	154.4	164.8	-10.4
C_6H_6ClN	p-chloroaniline	147.3	137.2	10.1
$C_6H_8N_2$	1,3-phenylenediamine	159.4	130.5	28.9
$C_6H_{13}NO_2$	L-leucine	200.8	192.9	7.9
$C_6H_{13}NO_2$	6-aminohexanoic acid	175.7	209.2	-33.5

$C_6H_{13}NO_2$	DL-leucine	194.1	192.9	1.2
$C_6H_{13}NO_2$	L-isoleucine	188.3	192.9	-4.6
$C_7H_7NO_2$	2-aminobenzoic acid	165.3	161.9	3.4
$C_7H_7NO_2$	3-aminobenzoic acid	162.8	161.9	0.9
$C_7H_7NO_2$	4-aminobenzoic acid	177.8	161.9	15.9
C_7H_9N	4-methylaniline	124.3	145.2	-20.9
C_7H_9NO	p-anisidine	236.0	195.0	41.0
$C_8H_{17}NO_2$	8-aminooctanoic acid	251.9	263.2	-11.3
$C_9H_9NO_2$	m-aminocinnamic acid	227.6	217.1	10.5
$C_9H_{11}NO_2$	L-phenylalanine	202.9	206.7	-3.8
$C_9H_{11}NO_3$	L-tyrosine	216.3	221.3	-5.0
$C_{10}H_9N$	2-naphthylamine	125.9	169.9	-44.0
$C_{12}H_{12}N_2O$	4,4'diaminodiphenyl ether	278.2	267.4	10.8
$C_{12}H_{14}N_4O$	3,3',4,4'tetraaminodiphenyl ether	319.7	292.5	27.2
$C_{13}H_{14}N_2$	*bis*-(4-aminophenyl)methane	270.7	244.3	26.4
$C_{13}H_{14}N_2O_2$	*bis*-(3-hydroxy-4-amino-phenyl)methane	281.2	273.2	8.0
$C_8H_9NO_2$	D-α-phenylglycine	177.4	179.9	-2.5

Parameters derived from the correlations:	Group	Entries
primary amines (c):	21.6	38
ethers (c):	49.8	8
nitro groups (c):	56.1	26

Solid Nitriles

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_3H_2N_2$	dicyanomethane	110.5	111.7	-1.2
$C_5H_6N_2$	2,2-dicyanopropane	179.5	152.7	26.8
$C_8H_4N_2$	1,2-dicyanobenzene	161.5	171.5	-10.0
$C_8H_4N_2$	1,4-dicyanobenzene	161.1	171.5	-10.4
$C_8H_{11}N$	*exo*-2-cyanobicyclo[2.2.1] heptane	200.0	175.7	24.3
$C_8H_{11}N$	*endo*-2-cyanobicyclo[2.2.1] heptane	194.1	175.7	18.4
$C_{10}H_2N_4$	1,2,4,5-tetracyanobenzene	222.2	238.5	-16.3
$C_{17}H_{14}N_2$	2,2-bis-(4-cyanophenyl) propane	355.6	327.2	28.4

Parameter derived from the correlation:	Group	Entries
nitriles (c):	42.3	8

Solid Isocyanates

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_8H_4N_2O_4$	1,4-diisocyanatobenzene	211.7	192.9	18.8
$C_{12}H_6N_2O_2$	1,5-naphthalenediisocyanate	223.4	244.8	-21.4

$(C_{15}H_{10}N_2)_2$	bis (4-isocyanatophenyl) methane	307.1	306.7	0.4

Parameter derived from the correlation:	Group	Entries
isocyanates (s):	[52.7]	3

Solid Tertiary Cyclic sp^2 Nitrogen

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_3H_3N_3$	s-triazine	95.4	94.6	0.8
$C_3H_3N_3O_3$	s-triazine triol	133.5	137.7	-4.2
$C_4H_4N_2$	pyrazine*	179.9	97.9	82.0
$C_6H_3C_{14}N$	2-chloro-1-(trichloromethyl) pyridine	192.0	193.3	-1.3
C_9H_7N	isoquinoline	177.8	153.6	24.2
$C_{13}H_9N$	7,8-benzoquinoline	206.3	205.9	0.4
$C_{13}H_9N$	acridine	205.0	205.9	-0.9
$C_{13}H_9N$	phenanthridine	201.7	205.9	-4.2
$C_{21}H_{15}N_3$	triphenyl-s-triazine	345.2	355.6	-10.4
$C_{23}H_{17}N$	2,4,6-triphenylpyridine	358.6	362.8	-4.2

Parameter derived from the correlation:	Group	Entries
cyclic tertiary sp^2 nitrogen (c):	13.9	9

*Not used in the correlation

Solid Tertiary sp^2 Nitrogen

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_8H_{12}N_4$	2,2'azodiisobutyrodinitrile	238.1	242.3	-4.2
$C_{12}H_{10}N_2$	*trans*-azobenzene	229.3	213.8	15.5
$C_{18}H_{21}NO$	N-(4-methoxybenzylidene)-p-butylaniline	451.0	410.0	41.0
$C_{18}H_{21}NO$	N-(2-hydroxy-4-methoxy-benzylidene)-p-butylaniline	451.0	424.7	26.3
$C_{19}H_{22}ClNO$	p-n-hexyloxybenzylideneamino-p'-chlorobenzene	435.1	456.1	-21.0
$C_{19}H_{23}NO$	N-p-ethoxybenzylidene-p'-butylaniline	429.3	436.8	-7.5
$C_{20}H_{25}NO$	p-n-hexyloxybenzylidene-p'-toluidine	441.4	464.0	-22.6
$C_{20}H_{22}N_2O$	p-n-hexyloxybenzylideneamino-p'-benzonitrile	432.6	469.9	-37.3
$C_{22}H_{29}NO$	N-p-n-pentyloxybenzylidene-p'-n-butylaniline	478.2	518.0	-39.8
$C_{23}H_{31}NO$	N-p-n-hexyloxybenzylidene-p'-n-butylaniline	512.1	544.8	-32.7

Parameter derived from the correlation:	Group	Entries
tertiary sp^2 nitrogen (c):	10.7	10

Solid Cyclic Tertiary sp^3 Nitrogen

	Compounds	Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_3H_6N_6O_6$	1,3,5-trinitro-1,3,5-triazacyclohexane	248.9	245.6	3.3
$C_4H_8N_8O_8$	α-1,3,5,7-tetra nitro-1,3,5,7-tetrazocine	307.1	327.6	-20.5
$C_6H_{12}N_2$	1,4-diazabicyclo[2.2:2] octane	153.1	150.2	2.9
$C_6H_{12}N_4$	1,3,5,7-tetraazatricyclo [3.3.1.1(3,7)]decane	152.3	152.3	0.0
$C_7H_{13}N$	1-azabicyclo[2.2.2]octane	169.5	152.3	17.2
$C_8H_{18}N_2O_2$	*bis*-hydroxyethylpiperazine	250.6	255.6	-5.0
$C_{13}H_{11}N$	N-methylcarbazole	218.0	212.1	5.9
$C_{19}H_{14}N_2$	1,2-diphenylbenzimidazole	318.8	299.2	19.6

Solid Cyclic Secondary sp^3 Nitrogen

	Compounds	Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_2H_3N_3$	1,2,4-triazole	78.7	83.7	-5.0
$C_5H_5N_5$	adenine	146.9	146.4	0.5
$C_6H_5N_3$	benzotriazole	178.7	138.9	39.8
$C_7H_6N_2$	benzimidazole	128.9	141.0	-12.1
$C_7H_6N_2$	indazole	128.9	141.0	-12.1
C_8H_7N	indole	192.0	142.7	49.3
$C_8H_{15}N$	3-azabicyclo[3.2.2]nonane	238.9	195.0	43.9
$C_{11}H_{12}N_2O_2$	L-tryptophane	238.1	242.3	-4.2
$C_{16}H_{36}N_4$	*cis*-(5,12)-7,7,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane	444.8	498.3	-53.5

Solid Secondary Amines

	Compounds	Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_3H_7NO_2$	N-methylglycine	128.9	116.3	12.6
$C_4H_{11}NO_2$	diethanolamine C	136.8	154.4	-17.6
$C_{24}H_{22}N_4O$	4,4'dianilino-3,3'-diaminodiphenyl oxide	458.1	441.0	17.1

Parameters derived from the correlation:	Group	Entries
cyclic secondary sp^3 nitrogen (c):	23.9	9
cyclic tertiary sp^3 nitrogen (c):	1.21	7
secondary sp^3 nitrogen (c):	[-0.29]	3

Solid Primary Amides

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
C_2H_5NO	acetamide	90.4	91.2	-0.8
$C_4H_8N_2O_2$	succinamide	174.1	163.2	10.9
$C_4H_8N_2O_3$	L-asparagine	159.8	165.3	-5.5
$C_{11}H_{17}NO$	1-adamantyl carboxamide	220.5	243.5	-23.0

Parameter derived from the correlation:	Group	Entries
primary amide (s):	[54.4]	4

Solid Secondary Amides

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_2H_4N_2O_2$	diformylhydrazine	99.2	88.7	10.5
$C_4H_8N_2O_3$	glycylglycine	164.0	172.8	-8.8
$(C_6H_{11}NO)_n$	poly-ε-caprolactam	169.9	179.1	-9.2
$C_6H_{13}NO$	2,2,N-trimethylpropanamide	182.8	185.8	-3.0
$C_6H_{13}NO$	N-t-butylacetamide	190.0	185.8	4.2
C_8H_9NO	acetanilide	179.5	177.0	2.5
$C_8H_9NO_2$	o-hydroxyacetanilide	182.4	191.6	-9.2
$C_8H_9N_2O$	p-nitroacetanilide	230.5	224.3	6.2
$C_9H_9NO_3$	benzoylglycine	214.2	220.5	-6.3
$C_{19}H_{16}N_2O$	N-benzoyl-o-amino diphenylamine	356.5	323.4	33.1
$C_{11}H_{12}N_2O_4$	hippurylglycine	277.4	291.6	-14.2
$C_{22}H_{20}N_2O_4$	N,N'-bis(m-methoxyphenyl) terephthalamide	458.1	523.0	-64.9
$C_{22}H_{20}N_2O_4$	N,N'-bis(p-methoxyphenyl) terephthalamide	467.8	523.0	-55.2

Parameter derived from the correlation:	Group	Entries
secondary amides (c):	44.4	13

Solid Tertiary Amides

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_8H_{10}N_4O_2$	caffeine	231.8	253.6	-21.8
$C_{11}H_{12}N_2O$	antipyrine	268.2	243.5	24.7
$C_{11}H_{13}N_3O$	4-aminoantipyrene	294.6	254.0	40.6

Parameter derived from the correlation:	Group	Entries
cyclic tertiary amide (c):	[52.7]	3

Solid Tertiary Amines

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_{11}H_{14}N_2$	3-dimethylaminomethyl indole	283.7	263.2	20.5
$C_{18}H_{15}N$	triphenylamine	297.5	320.1	-22.6

Parameter derived from the correlation:	Group	Entries
tertiary sp^3 nitrogen (c):	[31.5]	2

Solid Carbamates

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_9H_{11}NO_2$	ethyl phenylcarbamate	227.2	235.6	-8.4
$C_{10}H_{13}NO_2$	propyl N-phenyl carbamate	263.6	262.8	0.8
$C_{13}H_{19}NO_2$	hexyl N-phenylcarbamate	336.8	343.5	-6.7
$C_{16}H_{25}N$	nonyl phenylcarbamate	471.1	424.3	46.8

Parameter derived from the correlation:	Group	Entries
carbamates (c):	[76.1]	4

Solid Cyclic Ethers

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_4H_8O_4$	tetroxane	142.3	137.2	5.1
$C_5H_{10}O_5$	pentacycloformaldehyde	171.5	171.5	0.0
$C_5H_{10}O_5$	xylose	184.1	198.7	-14.6
$C_5H_{10}O_5$	L-arabinose	184.1	198.7	-14.6
$C_5H_{10}O_5$	D-arabinose	184.1	198.7	-14.6
$C_5H_{10}O_5$	D-ribose	187.0	198.7	-11.7
$C_6H_{12}O_6$	L-sorbose (cyclic)	228.4	220.1	8.3
$C_6H_{12}O_6$	D-fructose	231.8	224.3	7.5
$C_6H_{12}O_6$	α-D-glucose	221.8	212.5	9.3
$C_6H_{12}O_6$	α-D-galactose	216.3	212.5	3.8
$C_6H_{12}O_6$	D-mannose	215.9	212.5	3.4
$C_6H_{12}O_6$	meso inositol	218.4	211.3	7.1
$C_{12}H_{22}O_{11}$	β-lactose	408.4	428.0	-19.6
$C_{12}H_{22}O_{11}$	maltose	434.7	428.0	6.7
$C_{12}H_{22}O_{11}$	sucrose	425.5	437.6	-12.1
$C_{31}H_{52}O_3$	α-tocopherol acetate	897.9	755.2	142.7

Parameter derived from the correlation:	Group	Entries
cyclic ether (c):	9.71	16

Solid Lactones

Compounds		Heat Capacities J/(K mole) C_p(c) Expt	C_p(c) Calc	Expt-Calc
$C_4H_4O_4$	ethylene oxalate	141.8	139.7	2.1
$C_4H_4O_4$	1,4-dioxane-2,5-dione	133.5	139.7	-6.2
$C_6H_8O_4$	DL lactide	184.1	187.0	-2.9
$C_{13}H_{24}O_2$	tridecanolactone	398.3	340.2	58.1
$C_{15}H_{28}O_2$	pentadecanolactone	444.3	389.5	54.8

Parameter derived from the correlation:	Group	Entries
lactone (c):	[45.2]	5

Solid Aldehydes

Compounds		Heat Capacities J/(K mole) C_p(c) Expt	C_p(c) Calc	Expt-Calc
$C_7H_6O_3$	3,4-dihydroxybenzaldehyde	205.9	209.2	-3.3
C_9H_7NO	3-indole aldehyde	220.5	215.9	4.6

Parameter derived from the correlation:	Group	Entries
solid aldehydes (c):	[84.5]	2

Solid Ketones

Compounds		Heat Capacities J/(K mole) C_p(c) Expt	C_p(c) Calc	Expt-Calc
C_3H_6O	acetone	96.2	101.3	-5.1
$C_{13}H_{20}O$	4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	382.8	306.7	76.1
$C_{14}H_{10}O_2$	benzil	245.6	248.5	-2.9
$C_{14}H_{28}O$	2-tetradecanone	415.1	397.5	17.6
$C_{15}H_{30}O$	2-pentadecanone	426.8	424.7	2.1

Parameter derived from the correlation:	Group	Entries
ketone (c):	[28.0]	5

Solid Cyclic Ketones

Compounds		Heat Capacities J/(K mole) C_p(c) Expt	C_p(c) Calc	Expt-Calc
$C_4H_2O_4$	squaric acid	121.8	125.1	-3.3
$C_6Cl_4O_2$	tetrachlorobenzoquinone	193.7	202.1	-8.4
$C_6H_4O_2$	p-quinone	126.4	132.2	-5.8
$C_6H_8O_2$	1,4-cyclohexanedione	161.5	166.9	-5.4
$C_{10}H_{16}O$	(D) camphor	242.7	241.8	0.9

$C_{10}H_{16}O$	(DL) camphor	271.1	241.8	29.3
$C_{14}H_8O_2$	anthraquinone	240.2	242.7	-2.5
$C_{29}H_{42}O_2$	2,6-di-t-butyl-4-(3,5-ditert-butyl-4-oxocyclohexa-2,5-dienylidene methyl)phenol	654.0	615.5	38.5

Parameters derived from the correlation: Group Entries
cyclic ketone (c): 34.3 8

Solid Fluorides

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_6H_2F_5N$	pentafluoroaniline	231.0	196.6	34.4
$C_{12}H_8F_2$	4,4'difluorobiphenyl	222.6	223.8	-1.2
$C_{12}F_{10}$	perfluorobiphenyl	317.6	349.8	-32.2
$C_{19}H_{22}FNO$	p-n-hexyloxybenzylideneamino-p'-fluorobenzene	442.7	452.3	-9.6

Parameter estimated from the correlation: Group Entries
fluorides (c): [24.8] 4

Solid Quaternary Silanes

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_6H_{16}Si_2$	1,1,3,3-tetramethyl-1,3-disilacyclobutane	216.7	260.2	-43.5
$C_7H_{20}Si_2$	hexamethyldisilylmethane	357.3	311.3	46.0
$C_8H_{24}Si_4N_4$	octamethyltetrasilazane	569.9	518	51.9
$C_9H_{24}Si_2$	1,3-bis(trimethylsilyl) propane	394.1	365.3	29.3
$C_9H_{24}Si_3$	1,1,3,3,5,5-hexamethyl-1,3,5-trisilacyclohexane	400.8	390.8	10.5
$(C_{10}H_{14}Si)_n$	polyvinyldimethylphenyl-silane	231.0	237.7	-6.7
$(C_{11}H_{16}Si)_n$	polyvinyldimethylbenzyl-silane glass	310.5	264.5	46.0
$C_{12}H_9Cl_3Si$	p-trichlorosilylbiphenyl	291.2	301.7	-10.5
$C_{16}H_{12}Si$	diethynyldiphenylsilane	382.0	329.7	51.9
$C_{18}H_{15}ClSi$	triphenylchlorosilane	336.8	349.4	-12.6
$C_{18}H_{28}Si_4O_4$	1,1,3,3,5,5-hexamethyl-7,7-diphenyltetrasiloxane	633.0	580.3	52.7
$C_{21}H_{24}Si_3O_3$	*cis*-tri(methylphenyl)-trisiloxane	538.5	524.7	13.8
$C_{21}H_{24}SiO_3$	*trans*-tri(methylphenyl)-trisiloxane	506.7	524.7	-18.0
$C_{28}H_{32}Si_4O_4$	tetra(methylphenyl) tetrasiloxane	615.0	699.6	-84.5
$C_{38}H_{36}O_4Si_4$	1,1,3,3,5,5-hexaphenyl-7,7-dimethylcyclotetrasiloxane	815.5	818.4	-2.9

$C_{48}H_{40}O_4Si_4$	octaphenyl-cyclotetrasiloxane	932.6	937.6	-5.0

Parameter estimated from the correlation:	Group	Entries
quaternary silicon (c):	32.4	16

Solid Anhydrides

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_4H_2O_3$	maleic anhydride	120.1	112.1	8.0
$C_8H_4O_3$	phthalic anhydride	159.8	167.4	-7.6
$C_8H_{10}O_3$	*cis*-cyclohexane-1,2-dicarboxylic anhydride	207.5	202.1	5.4
$C_9H_8O_3$	*endo*-bicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid anhydride	183.3	183.7	-0.4
$C_{10}H_2O_6$	pyromellitic dianhydride	220.1	229.7	-9.6

Parameter estimated from the correlation:	Group	Entries
cyclic anhydrides (s):	[80.3]	6

Cyclic Secondary Amides

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_4H_5N_3O$	cytosine	132.6	118.8	13.8
$C_4H_6N_2O_2$	2,5-dioxopiperazine	133.9	142.3	-8.4
$C_4H_4N_2O_2$	uracil	120.5	125.1	-4.6
$C_5H_4N_4O$	hypoxanthine	134.3	139.7	-5.4
$C_5H_4N_4O$	xanthine	151.5	153.1	-1.6
$C_5H_7N_2O_2$	thymine	150.2	150.2	0.0
C_5H_9NO	α-piperidone	208.4	144.8	63.6
$C_6H_{11}NO$	ε-caprolactam	156.9	169.5	-12.6
$C_7H_{13}NO$	ζ-enantholactam	205.0	194.1	10.9

Parameter estimated from the correlation:	Group	Entries
cyclic secondary amide (c):	46.4	9

Solid Mono Substituted Ureas

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_6H_{13}N_3O_3$	*dl*-citrulline	232.6	247.3	-14.7
$C_4H_6N_4O_3$	allantoin	179.9	187.9	-8.0
CH_3N_3O	semicarbazide	110.5	104.6	5.9

Parameter estimated from the correlation:	Group	Entries
mono subst urea (c):	[82.8]	3

Solid Mono Substituted Guanidines

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_4H_9N_3O_2$	creatine	184.5	176.1	8.4
$C_6H_{14}N_4O_2$	arginine	232.2	245.6	-13.4

Parameter estimated from the correlation:	Group	Entries
mono subst guanidine (c):	[59.4]	2

Solid Quaternary Tin Compounds

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_{20}H_{18}Sn$	triphenylvinyltin	486.6	433.0	53.6
$C_{26}H_{20}Sn$	triphenylphenylethynyltin	447.7	492.5	-45.2

Parameter estimated from the correlation:	Group	Entries
quaternary tin (c):	[77.2]	2

Cyclic Imides

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_4H_5NO_2$	succinimide	131.4	122.6	8.8
$C_4H_4N_2O_3$	barbituric acid	141.0	144.3	-3.3

Parameter estimated from the correlation:	Group	Entries
cyclic imide (c):	[74.1]	3

Solid Quaternary Germanium Compounds

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc	Expt-Calc
$C_{16}H_{12}Ge$	diethynyldiphenylgermane	307.1	316.3	-9.2
$C_{32}H_{22}Ge$	1,1-diethynyl-2,3,4,5-tetraphenyl-1-germacyclopentadiene	556.5	527.2	29.3

Parameter estimated from the correlation:	Group	Entries
quaternary germanium (c):	[18.9]	2

Miscellaneous Solids

Compounds		Heat Capacities J/(K mole) $C_p(c)$ Expt	$C_p(c)$ Calc
$C_3H_4O_3$	ethylene carbonate	117.6	118.0
$C_3H_7NO_2S$	L-cysteine	162.3	162.3
$C_5H_4N_4O_3$	uric acid	166.1	166.1
$C_5H_{11}NO_2S$	methionine	290.0	290.4
$C_6H_{12}N_2O_4S_2$	L-cystine	261.9	261.9
$C_8H_4Cl_2O_2$	terephthaloyl dichloride	207.9	207.5
$C_{12}H_8S$	dibenzothiophene	194.6	194.6
$C_{12}H_{10}SO$	diphenyl sulfoxide	239.7	240.2

Parameters estimated from the correlation:	Group	Entries
sulfides (c):	[116]	1
thiols (c):	[51.9]	1
cyclic sulfides (c):	[20.3]	1
acid chlorides (c):	[60.2]	1
sulfoxides (c):	[47.7]	1
cyclic carbonates (c):	[68.2]	1
cyclic urea (c):	[63.6]	1
disulfides (c):	[41.0]p	1