D-Alanine

Other names:	(S)-(+)-alanine
	(S)-2-aminopropanoic acid
	.alpha.-alanine
	Alanine, D-
	Ba 2776
	D(-)-«alpha»-Alanine
	D-(-)-Alanine
	D-«alpha»-Alanine
	L-.alpha.-aminopropionic acid
	L-2-aminopropanoic acid
	L-alanine
Inchi:	InChI=1S/C3H7NO2/c1-2(4)3(5)6/h2H,4H2,1H3,(H,5,6)/t2-/m0/s1
InchiKey:	QNAYBMKLOCPYGJ-REOHCLBHSA-N
Formula:	C3H7NO2
SMILES:	CC(N)C(=O)O
Mol. weight [g/mol]:	89.09
CAS:	338-69-2

Physical Properties

Property code	Value	Unit	Source
chs	-1623.00 ± 0.20	kJ/mol	NIST Webbook
chs	-1576.00 ± 3.50	kJ/mol	NIST Webbook
chs	-1619.60 ± 0.54	kJ/mol	NIST Webbook
chs	-1639.90	kJ/mol	NIST Webbook
gf	-227.35	kJ/mol	Joback Method
hf	-341.55	kJ/mol	Joback Method
hfs	-561.24 ± 0.59	kJ/mol	NIST Webbook
hfs	-605.00 ± 3.50	kJ/mol	NIST Webbook
hfus	10.89	kJ/mol	Joback Method
hvap	55.95	kJ/mol	Joback Method
log10ws	0.28		Crippen Method
logp	-0.582		Crippen Method
mcvol	70.550	ml/mol	McGowan Method
pc	6046.69	kPa	Joback Method
ss	132.20	J/mol×K	NIST Webbook
tb	486.18	K	Joback Method
tc	677.88	K	Joback Method

tf	302.58	K	Joback Method
vc	0.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.30	J/mol×K	486.18	Joback Method
cpg	157.40	J/mol×K	518.13	Joback Method
cpg	163.22	J/mol×K	550.08	Joback Method
cpg	168.75	J/mol×K	582.03	Joback Method
cpg	174.01	J/mol×K	613.98	Joback Method
cpg	179.00	J/mol×K	645.93	Joback Method
cpg	183.73	J/mol×K	677.88	Joback Method
cps	120.80	J/mol×K	296.80	NIST Webbook
hsubt	132.80	kJ/mol	416.50	NIST Webbook
hsubt	138.00 ± 8.00	kJ/mol	461.00	NIST Webbook

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Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume