Alanine

Other names:	(R)-(-)-alanine
	(R)-2-aminopropanoic acid
	(S)-2-Aminopropanoic acid
	(S)-Alanine
	2-Aminopropanoic acid
	2-Aminopropanoic acid, L-
	2-Aminopropionic acid
	ALPHA-ALANINE
	ALPHA-AMINOPROPIONIC ACID
	Ala
	Alanine, L-
	D-2-aminopropanoic acid
	D-alanine
	L-(+)-Alanine
	L-2-Aminopropanoic acid
	L-2-Aminopropionic acid
	L-Alanine
	L-CH3CH(NH2)COOH
	L-«alpha»-Alanine
	L-«alpha»-Aminopropionic acid
	L-Â«alphaÂ»-Alanine
	L-Â«alphaÂ»-Aminopropionic acid
	NSC 206315
	Propanoic acid, 2-amino-
	Propanoic acid, 2-amino-, (S)-
	Ritalanine
	propanoic acid, D-2-amino-
	«alpha»-Alanine
	«alpha»-Aminopropionic acid
	Â«alphaÂ»-Alanine
	Â«alphaÂ»-Aminopropionic acid
Inchi:	InChI=1S/C3H7NO2/c1-2(4)3(5)6/h2H,4H2,1H3,(H,5,6)/t2-/m1/s1
InchiKey:	QNAYBMKLOCPYGJ-UWTATZPHSA-N
Formula:	C3H7NO2
SMILES:	CC(N)C(=O)O
Mol. weight [g/mol]:	89.09
CAS:	56-41-7

Physical Properties

Property code	Value	Unit	Source
affp	901.60	kJ/mol	NIST Webbook
affp	894.50 ± 0.40	kJ/mol	NIST Webbook
affp	902.00 ± 4.00	kJ/mol	NIST Webbook
basg	863.60 ± 6.70	kJ/mol	NIST Webbook
basg	867.70	kJ/mol	NIST Webbook
basg	865.40 ± 0.40	kJ/mol	NIST Webbook
basg	864.00 ± 6.30	kJ/mol	NIST Webbook
chs	-1577.00 ± 2.00	kJ/mol	NIST Webbook
chs	-1621.00 ± 1.70	kJ/mol	NIST Webbook
chs	-1634.10	kJ/mol	NIST Webbook
chs	-1621.45 ± 0.48	kJ/mol	NIST Webbook
gf	-227.35	kJ/mol	Joback Method
hf	-414.70 ± 4.20	kJ/mol	NIST Webbook
hfs	-560.00 ± 1.70	kJ/mol	NIST Webbook
hfs	-559.48	kJ/mol	NIST Webbook
hfs	-562.70	kJ/mol	NIST Webbook
hfus	10.89	kJ/mol	Joback Method
hsub	144.80 ± 4.20	kJ/mol	NIST Webbook
hsub	144.80 ± 4.20	kJ/mol	NIST Webbook
hvap	55.95	kJ/mol	Joback Method
ie	8.88	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.88	eV	NIST Webbook
ie	9.63	eV	NIST Webbook
log10ws	0.27		Aqueous Solubility Prediction Method
logp	-0.582		Crippen Method
mcvol	70.550	ml/mol	McGowan Method
pc	6046.69	kPa	Joback Method
ss	118.80	J/mol×K	NIST Webbook
ss	129.21	J/mol×K	NIST Webbook
tb	486.18	K	Joback Method
tc	677.88	K	Joback Method
tf	555.82	K	Aqueous Solubility Prediction Method
vc	0.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.73	J/mol×K	677.88	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	151.30	J/mol×K	486.18	Joback Method
cps	115.00	J/mol×K	298.00	NIST Webbook
cps	115.20	J/mol×K	298.00	NIST Webbook
cps	122.26	J/mol×K	298.15	NIST Webbook
hsubt	133.00 ± 1.00	kJ/mol	414.00	NIST Webbook
hsubt	132.40 ± 1.30	kJ/mol	431.50	NIST Webbook
hsubt	138.00 ± 0.80	kJ/mol	455.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56417&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Activity coefficients of glycine, d-alanine and l-valine in aqueous solutions containing MgSO4 at 298.15 K: experimental determination and correlation: https://www.doi.org/10.1016/j.fluid.2011.10.015

Temperature Dependences and Enthalpic Discrimination of Homochiral Dimeric Interactions of Six a-Amino Acid Enantiomers in Pure Water: https://www.doi.org/10.1021/je500825a

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1465

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

affp: Proton affinity

basg: Gas basicity

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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