«beta»-Alanine

Other names:	.beta.-alanine
	2-Carboxyethylamine
	3-Aminopropanoic acid
	3-Aminopropionic acid
	Abufene
	Alanine, beta-
	Beta-alanine
	NSC 7603
	Propanoic acid, 3-amino-
	«beta»-Aminopropionic acid
	«omega»-Aminopropionic acid
	Â«betaÂ»-Aminopropionic acid
	Â«omegaÂ»-Aminopropionic acid
Inchi:	InChI=1S/C3H7NO2/c4-2-1-3(5)6/h1-2,4H2,(H,5,6)
InchiKey:	UCMIRNVEIXFBKS-UHFFFAOYSA-N
Formula:	C3H7NO2
SMILES:	NCCC(=O)O
Mol. weight [g/mol]:	89.09
CAS:	107-95-9

Physical Properties

Property code	Value	Unit	Source
chs	-1871.00 ± 1.50	kJ/mol	NIST Webbook
chs	-1622.90 ± 0.23	kJ/mol	NIST Webbook
gf	-224.91	kJ/mol	Joback Method
hf	-424.00 ± 2.00	kJ/mol	NIST Webbook
hfs	-547.10 ± 1.10	kJ/mol	NIST Webbook
hfs	-558.04 ± 0.31	kJ/mol	NIST Webbook
hfs	-310.00 ± 1.50	kJ/mol	NIST Webbook
hfus	14.41	kJ/mol	Joback Method
hsub	134.00 ± 2.00	kJ/mol	NIST Webbook
hsub	134.00 ± 2.00	kJ/mol	NIST Webbook
hvap	56.34	kJ/mol	Joback Method
log10ws	1.00		Aqueous Solubility Prediction Method
logp	-0.580		Crippen Method
mcvol	70.550	ml/mol	McGowan Method

pc	5972.16	kPa	Joback Method
tb	486.62	K	Joback Method
tc	674.22	K	Joback Method
tf	477.50	K	Thermophysical Study of Several alpha- and beta-Amino Acid Derivatives by Differential Scanning Calorimetry (DSC)
vc	0.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.00	J/mol×K	486.62	Joback Method
cpg	156.90	J/mol×K	517.89	Joback Method
cpg	162.53	J/mol×K	549.15	Joback Method
cpg	167.90	J/mol×K	580.42	Joback Method
cpg	173.01	J/mol×K	611.68	Joback Method
cpg	177.88	J/mol×K	642.95	Joback Method
cpg	182.49	J/mol×K	674.22	Joback Method
cps	109.00	J/mol×K	298.00	NIST Webbook
cps	109.30	J/mol×K	298.00	NIST Webbook
cps	116.40	J/mol×K	298.00	NIST Webbook
hsubt	133.10 ± 0.70	kJ/mol	393.00	NIST Webbook

Sources

Osmotic and activity coefficients of alpha, omega-amino acids in aqueous solutions at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2014.02.004
Partial Molar Volumes, Partial Molar Compressibilities, and Viscosities of alpha,ω-Amino Acids in Water and in Aqueous Sodium Chloride Solutions at 298.15 K:	https://www.doi.org/10.1021/acs.jced.8b00236
Binary Diffusion Coefficients of Aqueous Straight-Chain Amino Acids over a Temperature Range of 293.23 K to 343.23 K:	https://www.doi.org/10.1021/je301370s
Studies on the Diffusion Coefficients of Amino Acids in Aqueous Solutions: 298.2 to 333.2 K:	https://www.doi.org/10.1021/je049582g
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Effect of temperature on the dilution enthalpies of alpha,omega-amino acids in aqueous solutions:	https://www.doi.org/10.1016/j.jct.2011.04.019
Study of the thermodynamic properties of aqueous binary mixtures of glycine, L-alanine and L-alanine at 10 K intervals between 278.15 and 308.15 K:	https://www.doi.org/10.1016/j.jct.2011.09.016
Solution Thermodynamic Analysis of 4-(Aminomethyl)benzoic Acid in Four Neat Solvents from 288.15 to 328.15 K:	https://www.doi.org/10.1021/acs.jced.8b00763
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107959&Units=SI

Thermophysical Study of Several alpha- and beta-Amino Acid Derivatives by Differential Scanning Calorimetry (DSC):

https://www.doi.org/10.1021/je200292z

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
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume