dl-Alanine

Other names:	(.+/-.)-Alanine
	ALANINE, «alpha»
	Alanine, DL-
	DL-«alpha»-Alanine
	dl-2-aminopropanoic acid
	dl-«alpha»-Aminopropionic acid
Inchi:	InChI=1S/C3H7NO2/c1-2(4)3(5)6/h2H,4H2,1H3,(H,5,6)
InchiKey:	QNAYBMKLOCPYGJ-UHFFFAOYSA-N
Formula:	C3H7NO2
SMILES:	CC(N)C(=O)O
Mol. weight [g/mol]:	89.09
CAS:	302-72-7

Physical Properties

Property code	Value	Unit	Source
chs	-1602.00 ± 2.90	kJ/mol	NIST Webbook
chs	-1623.40 ± 0.20	kJ/mol	NIST Webbook
chs	-1617.30 ± 0.59	kJ/mol	NIST Webbook
chs	-1633.60	kJ/mol	NIST Webbook
gf	-227.35	kJ/mol	Joback Method
hf	-341.55	kJ/mol	Joback Method
hfs	-578.90 ± 2.90	kJ/mol	NIST Webbook
hfs	-563.63 ± 0.59	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	563.50	K	Thermophysical Study of Several alpha- and beta-Amino Acid Derivatives by Differential Scanning Calorimetry (DSC)

vc	0.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	157.40	J/mol×K	518.13	Joback Method
cpg	183.73	J/mol×K	677.88	Joback Method
cps	114.00	J/mol×K	298.00	NIST Webbook
cps	113.80	J/mol×K	298.00	NIST Webbook
cps	121.60	J/mol×K	298.15	NIST Webbook
cps	121.71	J/mol×K	297.50	NIST Webbook

Sources

Interactions of some ex-amino acids with tetra-n-alkylammonium bromides in aqueous medium at different temperatures:	https://www.doi.org/10.1016/j.jct.2006.08.010
Thermodynamics of the interactions of some amino acids and peptides with dodecyltrimethylammonium bromide and tetradecyltrimethylammonium bromide:	https://www.doi.org/10.1016/j.jct.2013.11.001
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Water Activity in Aqueous Amino Acid Solutions Containing Ammonium Sulfate at 298.2 K:	https://www.doi.org/10.1021/je401034k
Studies on the Diffusion Coefficients of Amino Acids in Aqueous Solutions:	https://www.doi.org/10.1021/je049582g
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of salicylic acid in pure alcohols at different temperatures:	https://www.doi.org/10.1016/j.jct.2012.09.006
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Partial Molar Volumes and Viscosities of Some r-Amino Acids in Micellar Solutions of Sodium Caprylate:	https://www.doi.org/10.1021/je049927v
Surface Tension of Glycine, Alanine, Aminobutyric Acid, Norvaline, and Norleucine in Water and in Aqueous Solutions of Strong Electrolytes at Temperature=Smooth (293.15 to 313.15)	https://www.doi.org/10.1021/acs.jced.7b00433
Volumetric properties of amino acids in aqueous solutions of ammonium based ionic liquids at T = (288.15 to 318.15) K	https://www.doi.org/10.1016/j.fluid.2014.11.016
Study of Interactions between Amino Acids and Zinc Chloride in Aqueous Solutions through Volumetric Measurements at T) (288.15 to 318.15)	https://www.doi.org/10.1021/je8001464
Solubility and Chemical Thermodynamics of dl-Alanine and Glycine in Aqueous NaCl and KCl Solutions:	https://www.doi.org/10.1021/acs.jced.5b00351
Standard molar enthalpy of formation of Nd(Gly)2(Ala)3Cl3*2H2O(s):	https://www.doi.org/10.1016/j.tca.2004.05.030
Volumetric and viscometric study of the ternary (dl-alanine/+d(-)-fructose + water) solution at different temperatures	https://www.doi.org/10.1016/j.jct.2018.06.008
Volumetric, ultrasonic, and viscometric behaviour of glycine, DL-alanine, and DL-2-aminobutyric acid in aqueous solutions at different temperatures	https://www.doi.org/10.1016/j.jct.2008.09.008
Effect of various DL-alanine and DL-2-aminobutyric acid on the isentropic and activity coefficients of glycine, dl-a-alanine and dl-a-aminobutyric acid in aqueous solutions at temperatures between 288.15 and 303.15 K:	https://www.doi.org/10.1016/j.jct.2015.04.024
Experimental and Transpheric Pressures of 1,4-Butanediol Solutions at different temperatures: Temperature of maximum density of water:	https://www.doi.org/10.1016/j.fluid.2006.10.012

Phase Equilibrium System of Cadmium Chloride + dl-Alanine + Water at 298.15 K and Standard Molar Enthalpy of Formation of Cd3(Ala)2Cl6*4H2O:	https://www.doi.org/10.1021/je900845g
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C302727&Units=SI
Thermophysical Study of Several alpha- and beta-Amino Acid Derivatives by Differential Scanning Calorimetry (DSC):	https://www.doi.org/10.1021/je200292z
Solubility and Solvation Thermodynamics of a Series of Homologous a-Amino Acids in Nonaqueous Binary Mixtures of Ethylene Glycol and Dimethyl Sulfoxide:	https://www.doi.org/10.1021/je5007899
The effect of ammonium sulfate on the solubility of amino acids in water at (298.15 and 323.15) K:	https://www.doi.org/10.1016/j.jct.2008.09.019
Solubility of triclosan and iodopropynyl butylcarbamate in pure alkanols at several temperatures:	https://www.doi.org/10.1016/j.fluid.2012.05.020
Effect of sodium caproate on the volumetric and viscometric properties of glycine, DL-alpha-alanine, and DL-alpha-amino-n-butyric acid in aqueous solutions:	https://www.doi.org/10.1016/j.jct.2003.11.001
Volumetric, viscometric, and refractive index behaviour of α-amino acids and their group contribution in aqueous D-glucose solution at different temperatures:	https://www.doi.org/10.1016/j.jct.2005.04.011
Excess Volume of Water in Hydrate Complexes of Some alpha-Amino Acids:	https://www.doi.org/10.1021/je400415r
Volumetric and Viscometric Studies of Some Amino Acids in Aqueous Solutions of Cadmium Chloride at T = (288.15 to 318.15) K and at Atmospheric Pressure:	https://www.doi.org/10.1021/je100909b
Solubility and Thermodynamics of Solute-Solvent Interactions of Some Amino Acids in Aqueous Sodium Bromide and Potassium Bromide Solutions:	https://www.doi.org/10.1021/acs.jced.7b00647
KCl effect on the solubility of five different amino acids in water:	https://www.doi.org/10.1016/j.fluid.2007.04.004

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
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