

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	-1633.60	kJ/mol	NIST Webbook
chs	-1623.40 ± 0.20	kJ/mol	NIST Webbook
chs	-1617.30 ± 0.59	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/molxK	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)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.30	J/molxK	486.18	Joback Method
cpg	157.40	J/molxK	518.13	Joback Method
cpg	163.22	J/molxK	550.08	Joback Method
cpg	168.75	J/molxK	582.03	Joback Method
cpg	174.01	J/molxK	613.98	Joback Method
cpg	179.00	J/molxK	645.93	Joback Method
cpg	183.73	J/molxK	677.88	Joback Method
cps	114.00	J/molxK	298.00	NIST Webbook
cps	113.80	J/molxK	298.00	NIST Webbook
cps	121.60	J/molxK	298.15	NIST Webbook
cps	121.71	J/molxK	297.50	NIST Webbook

Sources

Surface Tension of Glycine, Alanine, Aminobutyric Acid, Norvaline, and Alanine in the Diffusion Coefficients of Amino Acids in Aqueous Solutions: Effect of glycine, DL-alanine and DL-2-aminobutyric acid on the temperature of maximum density of alcohols at different temperatures: Thermophysical Study of Several alpha- and beta-Amino Acid Derivatives by Density and Thermodynamic Property-Solvent Interactions of Some Amino Acids in Aqueous Solutions with NaCl and Potassium Iodide Solutions: Medium at different temperatures: The effect of ammonium sulfate on the solubility of amino acids in water at 298.15 and 303.15 K Water in Hydrate Complexes of Some alpha-Amino Acids Crippen Method:

Solubility and Chemical Thermodynamics of d,l-Alanine and d,l-Valine Interactions between Amino Acids and Zinc Chloride in Aqueous Solutions: Thermodynamic and viscometric behavior of glycine, DL-alanine and L-histidine in the interactions of some amino acids and peptides with dodecyltrimethylammonium bromide chloride and Alanine in Water at 298.15 K and 303.15 K: Thermodynamic Properties of Alanine in Aqueous Solutions: Containing Amino Acids: Barial Mol 2003/2 Kmes and Viscosities of Some r-Amino Acids in Micellar Solution of Sodium Caprylate: the volumetric and viscometric properties of glycine, DL-alpha-alanine, and DL-alpha-amino-n-butyric acid in aqueous solutions:

<https://www.doi.org/10.1021/acs.jced.7b00433>

<https://www.doi.org/10.1021/je049582g>

<https://www.doi.org/10.1016/j.jct.2015.04.024>

<https://www.doi.org/10.1016/j.jct.2012.09.006>

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

<https://www.doi.org/10.1021/acs.jced.7b00647>

<https://www.doi.org/10.1016/j.jct.2006.08.010>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C302727&Units=SI>

<https://www.doi.org/10.1016/j.jct.2008.09.019>

<https://www.doi.org/10.1021/je400415r>

https://www.chemeo.com/doc/models/crippen_log10ws

<https://www.doi.org/10.1021/acs.jced.5b00351>

<https://www.doi.org/10.1021/je8001464>

<https://www.doi.org/10.1016/j.jct.2008.09.008>

<https://www.doi.org/10.1016/j.jct.2013.11.001>

<https://www.doi.org/10.1021/je900845g>

<https://www.doi.org/10.1021/je401034k>

<https://www.doi.org/10.1021/je049927v>

<https://www.doi.org/10.1016/j.jct.2003.11.001>

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Volumetric and Viscometric Studies of Some Amino Acids in Aqueous Solutions of Calcium Chloride at T = (288.15 to 318.15) K and at Atmospheric Pressure	https://www.doi.org/10.1021/je100909b
McGowan Method	http://link.springer.com/article/10.1007/BF02311772
Polymetric, viscometric, and refractive index behaviour of α-amino acids and their groups and viscometric study of the ternary (dl-alanine/dl-erythro-fructose + Carboxylates) at different temperatures	https://www.doi.org/10.1016/j.jct.2005.04.011
Solubility of triclosan and iodopropynyl butylcarbamate in pure alkanols at several temperatures	https://www.doi.org/10.1016/j.jct.2018.06.008
Thermodynamics of a Series of Standard Solid Enthalpies of Formation of Amino Acids in Aqueous Solutions	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic Properties of Amino Acids in Aqueous Solutions of Ammonium Based Buffers and Activity Coefficients of glycine, dl-α-alanine and dl-α-amino butyric acid at different temperatures at 288.15 and 303.15 K:	https://www.doi.org/10.1016/j.fluid.2012.05.020
	https://www.doi.org/10.1021/je5007899
	https://www.doi.org/10.1016/j.tca.2004.05.030
	https://www.doi.org/10.1016/j.fluid.2014.11.016
	https://www.doi.org/10.1016/j.fluid.2006.10.012
	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

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