L-Alanine

Other names:	(S)-(+)-alanine (S)-2-aminopropanoic acid (S)-Alanine .alpha.-alanine 2-Aminopropanoic acid 2-Aminopropanoic acid, L- 2-Aminopropionic acid ALPHA-ALANINE ALPHA-AMINOPROPIONIC ACID Ala Alanine, L- L-(+)-Alanine L-.alpha.-aminopropionic acid L-2-Aminopropionic acid L-2-aminopropanoic acid L-CH3CH(NH2)COOH L-«alpha»-Alanine L-«alpha»-Aminopropionic acid NSC 206315 Propanoic acid, 2-amino- Propanoic acid, 2-amino-, (S)- Ritalanine «alpha»-Alanine «alpha»-Aminopropionic acid 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:	C[C@H](N)C(=O)O
Mol. weight [g/mol]:	89.09
CAS:	56-41-7

Physical Properties

Property code	Value	Unit	Source
af	0.6149		Cheméo Relay (1.0)
affp	894.50 ± 0.40	kJ/mol	NIST Webbook

affp	901.60	kJ/mol	NIST Webbook
affp	902.00 ± 4.00	kJ/mol	NIST Webbook
basg	865.40 ± 0.40	kJ/mol	NIST Webbook
basg	863.60 ± 6.70	kJ/mol	NIST Webbook
basg	864.00 ± 6.30	kJ/mol	NIST Webbook
basg	867.70	kJ/mol	NIST Webbook
chs	-1621.00 ± 1.70	kJ/mol	NIST Webbook
chs	-1621.45 ± 0.48	kJ/mol	NIST Webbook
chs	-1577.00 ± 2.00	kJ/mol	NIST Webbook
chs	-1634.10	kJ/mol	NIST Webbook
hf	-414.70 ± 4.20	kJ/mol	NIST Webbook
hfs	-560.00 ± 1.70	kJ/mol	NIST Webbook
hfs	-562.70	kJ/mol	NIST Webbook
hfs	-559.48	kJ/mol	NIST Webbook
hfus	15.34	kJ/mol	Joback Method
hsub	144.80 ± 4.20	kJ/mol	NIST Webbook
hsub	144.80 ± 4.20	kJ/mol	NIST Webbook
hvap	56.21	kJ/mol	Cheméo Relay (1.0)
ie	8.88	eV	NIST Webbook
ie	9.63	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.88	eV	NIST Webbook
log10ws	0.27		Aqueous Solubility Prediction Method
logp	-0.582		Crippen Method
mcvol	70.550	ml/mol	McGowan Method
pc	5470.75	kPa	Joback Method
ss	129.21	J/mol×K	NIST Webbook
ss	118.80	J/mol×K	NIST Webbook
tb	469.05	K	Cheméo Relay (1.0)
tc	637.05	K	Cheméo Relay (1.0)
tf	555.82	K	Aqueous Solubility Prediction Method
tf	570.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	0.260	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	9.57000e+00
Coeff. B	4.07420e-01
Coeff. C	-2.58600e-04
Coeff. D	6.30000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Study of solvation consequences of alpha-amino acids in aqueous ionic liquid solution probed by physicochemical approach:	https://www.doi.org/10.1016/j.fluid.2013.03.030
Apparent Molar Volumes and Viscosity B-Coefficients of Some Amino Acids in Aqueous Tetramethylammonium Iodide Solutions at 298.15 K: Temperature dependence and ion-group additivity	https://www.doi.org/10.1021/je7001418
Volumetric properties of glycine, L-alanine, L-valine in aqueous solutions of norfloxacin hydrochloride at different temperatures: An electrolyte compressibility study.	https://www.doi.org/10.1016/j.jct.2018.09.026
Volumetric, viscometric and ultrasonic studies of some amino acids in aqueous streptomycin sulfate solutions at different temperatures.	https://www.doi.org/10.1016/j.jct.2016.03.045
Thermodynamic interactions of amino acids from water to aqueous solutions of N-methylacetamide and 9 temperatures: Part 1. Glycine, L-alanine and L-serine in aqueous potassium chloride solutions.	https://www.doi.org/10.1016/j.tca.2008.10.023
Interaction of homologous series of amino acids with carnosine in presence of glycine, L-alanine and L-valine with aqueous solutions of trisodium citrate at different temperatures: A volumetric and acoustic approach.	https://www.doi.org/10.1016/j.jct.2015.11.015
Molecular interactions of some amino acids in methanol: A volumetric approach:	https://www.doi.org/10.1021/je5003797
A calorimetric study of interactions of amino acids with sodium 1-butyl-3-methylimidazolium bromide ionic liquid at 298.15K: Volumetric, viscometric and calorimetric approach:	https://www.doi.org/10.1016/j.tca.2008.10.011
Viscosity studies of (L-alanine-, L-proline-, L-valine-, L-serine-, L-leucine) in aqueous solutions of trimethylamine N-oxide at 298.15 K	https://www.doi.org/10.1016/j.tca.2004.05.021
Thermodynamic properties of the interactions of glycine, L-alanine and L-proline with aqueous solutions of sodium chloride at 298.15 K: Volumetric, viscometric and calorimetric studies	https://www.doi.org/10.1016/j.jct.2013.08.010
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Molecular interactions of some amino acids in methanol: A volumetric approach:	https://www.doi.org/10.1016/j.jct.2018.05.008
A calorimetric study of interactions of amino acids with sodium 1-butyl-3-methylimidazolium bromide ionic liquid at 298.15K: Volumetric, viscometric and calorimetric approach:	https://www.doi.org/10.1016/j.tca.2008.09.001
Viscosity studies of (L-alanine-, L-proline-, L-valine-, L-leucine) in aqueous solutions of trimethylamine N-oxide at 298.15 K	https://www.doi.org/10.1016/j.jct.2008.07.019
Thermodynamic properties of the interactions of glycine, L-alanine and L-proline with aqueous solutions of sodium chloride at 298.15 K: Volumetric, viscometric and calorimetric studies	https://www.doi.org/10.1016/j.jct.2011.05.012
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Physicochemical study of solute-solute and solute-solvent interactions of glycine, L-alanine, L-valine and	https://www.doi.org/10.1016/j.jct.2016.03.012
Low-temperature heat capacities and standard molar enthalpy of formation	https://www.doi.org/10.1016/j.tca.2008.02.024
Studies on the Diffusion Coefficients of Amino Acids in Aqueous Solutions	https://www.doi.org/10.1021/je049582g
Thermodynamics of (solute + solute) and (solute + solvent) interactions of	https://www.doi.org/10.1016/j.jct.2016.06.026
Study of the interactions of PAMAM-NH2 G4 dendrimer with	https://www.doi.org/10.1016/j.jct.2013.10.022
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Effect of 1-Ethyl-3-methylimidazolium	https://www.doi.org/10.1021/je300953u
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Transfer Enthalpies of Amino Acids	https://www.doi.org/10.1016/j.tca.2014.04.013
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Infinite Dilution Binary Diffusion	https://www.doi.org/10.1021/je060149b
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Physicochemical Properties of	https://www.doi.org/10.1007/s10765-011-1060-5
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Effect of NaBr, KCl, KBr, and MgCl2 on	https://www.doi.org/10.1021/je050048y
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Water Activity in Aqueous Amino Acid	https://www.doi.org/10.1021/je700466s
Measuring and modeling aqueous	https://www.doi.org/10.1016/j.jct.2013.08.018
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Thermodynamic Modeling of (CaCl2 +	https://www.doi.org/10.1021/acs.jced.5b00260
Transfer Partial Molar Isentropic	https://www.doi.org/10.1007/s10765-013-1432-0
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DL-serine, DL-threonine, L-histidine, L-asparagine, and L-glutamine at temperatures from (278.15 to 333.15) K, https://www.doi.org/10.1016/j.jct.2017.12.010

molalities from (0.0075 to 1.0) mol·kg-1, and at the pressure 0.99 MPa: Apparent

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Investigation on solute-solvent interactions of glycine, L-alanine and L-valine in aqueous tetraethylammonium chloride solutions at different temperatures with reference to theoretical models.	https://www.doi.org/10.1016/j.jct.2015.08.009
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Thermodynamic Study of Some Amino Acids, 2-Aminopropanoic Acid, 2-Amino-3-methylbutanoic Acid, and 2-Amino-3-phenylpropanoic Acid, in Aqueous Saccharide Solutions at Different Temperatures: Volumetric and Ultrasonic Study.	https://www.doi.org/10.1016/j.jct.2011.01.004
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	https://www.doi.org/10.1016/j.jct.2017.02.021
	https://www.doi.org/10.1016/j.fluid.2008.02.015

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
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

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