D-Alanine

Other names:	(S)-(+)-alanine
	(S)-2-aminopropanoic acid
	.alpha.-alanine
	Alanine, D-
	Ba 2776
	D(-)-«alpha»-Alanine
	D-(-)-Alanine
	D-«alpha»-Alanine
	L-.alpha.-aminopropionic acid
	L-2-aminopropanoic acid
	L-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:	CC(N)C(=O)O
Mol. weight [g/mol]:	89.09
CAS:	338-69-2

Physical Properties

Property code	Value	Unit	Source
chs	-1576.00 ± 3.50	kJ/mol	NIST Webbook
chs	-1619.60 ± 0.54	kJ/mol	NIST Webbook
chs	-1639.90	kJ/mol	NIST Webbook
chs	-1623.00 ± 0.20	kJ/mol	NIST Webbook
gf	-227.35	kJ/mol	Joback Method
hf	-341.55	kJ/mol	Joback Method
hfs	-605.00 ± 3.50	kJ/mol	NIST Webbook
hfs	-561.24 ± 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	302.58	K	Joback Method
vc	0.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	163.22	J/mol×K	550.08	Joback Method
cpg	168.75	J/mol×K	582.03	Joback Method
cpg	183.73	J/mol×K	677.88	Joback Method
cps	120.80	J/mol×K	296.80	NIST Webbook
hsubt	132.80	kJ/mol	416.50	NIST Webbook
hsubt	138.00 ± 8.00	kJ/mol	461.00	NIST Webbook

Sources

Volumetric Properties of Potassium Dihydrogen Citrate and Tripotassium Citrate in Water and in Aqueous Solutions of Alanine at T) (283.15 to 308.15) K:	https://www.doi.org/10.1021/je700288s
Effects of clustering structure on volumetric properties of amino acids in (DMSO + water) mixtures:	https://www.doi.org/10.1016/j.jct.2012.01.015
Effects of Concentration and Temperature on Interactions in (L-Alanine/ L-Threonine/ Glycylglycine + Aqueous Glucose/ Aqueous Sucrose) Systems: Insights from Viscosity Measurements:	https://www.doi.org/10.1016/j.tca.2013.11.006
Volumetric and Viscometric Studies of Amino Acids in Vitamin B6 Aqueous Solutions at Various Temperatures:	https://www.doi.org/10.1021/je500975a
Effect of NaBr, KCl, KBr, and MgCl2 on Viscosities of Aqueous Glycine and L-Alanine Solutions at 298.15 K:	https://www.doi.org/10.1021/je050048y
Effect of 1-Ethyl-3-methylimidazolium Bromide Ionic Liquid on the Volumetric Behavior of Some Aqueous L-Amino Acids Solutions:	https://www.doi.org/10.1021/je300953u
Partial molar volume and partial molar compressibility of four homologous alpha-amino acids in aqueous sodium fluoride solutions at different temperatures:	https://www.doi.org/10.1016/j.jct.2011.01.004
Viscosities of Glycine, L-Alanine, and L-Valine in (0.2, 0.4, 0.6, and 0.8) mol*kg-1 Aqueous Trisodium Citrate Solutions at Different Temperatures:	https://www.doi.org/10.1021/je400894j
Thermodynamic properties of 1-butyl-3-methylimidazolium salicylate as an active pharmaceutical ingredient ionic liquid (API-IL) in aqueous solutions of glycine and L-alanine at T = (288.15 to 318.15) K:	https://www.doi.org/10.1016/j.tca.2016.05.013
Effect of tetra-n-alkylammonium bromides on the volumetric properties of glycine, L-alanine and glycylglycine at T = (298.15 to 313.15) K:	https://www.doi.org/10.1016/j.jct.2003.09.008
Thermodynamics of the interactions of a homologous series of some amino acids with trimethylamine N-oxide: volumetric, compressibility, and calorimetric studies:	https://www.doi.org/10.1016/j.jct.2011.05.012
Physicochemical study of solute-solute and solute-solvent interactions of glycine, L-alanine, L-valine and L-isoleucine in aqueous-D-mannose solutions at temperatures from 293.15 K to 318.15 K:	https://www.doi.org/10.1016/j.jct.2016.03.012
Investigation of Volumetric and Acoustic Properties of Procainamide Hydrochloride in Aqueous Binary and (Water + Amino Acid) Ternary Mixtures at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.7b00452
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Effect of dipotassium hydrogen phosphate on thermodynamic properties of glycine and L-alanine in aqueous solutions at different temperatures:	https://www.doi.org/10.1016/j.jct.2012.04.020
Study of the interactions of PAMAM-NH2 G4 dendrimer with some essential amino acids in aqueous solutions:	https://www.doi.org/10.1016/j.jct.2013.10.022
Densities, Sound Speed, and Viscosities of Some Amino Acids with Aqueous Tetra-Butyl Ammonium Iodide Solutions at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.5b00198
Densities, Partial Molar Volumes, and Heat Capacities of Glycine, L-Alanine, and L-Leucine in Aqueous Magnesium Chloride Solutions at Different Temperatures:	https://www.doi.org/10.1021/je034168m
Enthalpies of transfer of amino acids from water to aqueous solutions of formamide:	https://www.doi.org/10.1016/j.tca.2005.04.002

Viscosities of Glycine and l-Alanine in (0.2, 0.4, 0.6, and 0.8) mol*kg 1 Aqueous Dipotassium Hydrogen Phosphate Solutions at Different Temperatures:	https://www.doi.org/10.1021/je300673m
Enthalpies of transfer of amino acids from water to aqueous solutions of sodium [illegible] and sodium perchlorate at T = 298.15K:	https://www.doi.org/10.1016/j.tca.2005.10.013
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Investigations on molecular interaction of some amino acids with the drug levofloxacin in aqueous solution by volumetric and acoustic methods at different temperatures:	https://www.doi.org/10.1016/j.jct.2016.09.027
Molecular interactions between some amino acids and a pharmaceutically active ionic liquid domiphen DL-mandelic acid in aqueous medium at temperatures from 293.15 K to 318.15 K:	https://www.doi.org/10.1016/j.jct.2019.06.002
Molecular interactions of some amino acids in aqueous 1-hexyl-3-methylimidazolium chloride solutions at different temperatures: A volumetric approach:	https://www.doi.org/10.1016/j.jct.2018.05.008
Volumetric Properties of Amino Acids in Aqueous N-Methylformamide Solutions at T = 298.15 K:	https://www.doi.org/10.1021/je1003466
Thermophysical Properties of 1-Hexyl-3-methylimidazolium Salicylate as an Active Pharmaceutical Ingredient Ionic Liquid (API-IL) in Aqueous Solutions of Glycine and l-Alanine:	https://www.doi.org/10.1021/acs.jced.8b00644
Study of thermodynamic properties of aqueous binary mixtures of glycine, L-alanine and L-serine at low temperatures (T = 275.15, 279.15, and 283.15) K:	https://www.doi.org/10.1016/j.jct.2011.09.016
Enthalpies of Transfer of Amino Acids from Water to Aqueous Solutions of Alkali Metal Nitrates:	https://www.doi.org/10.1021/je050296u
Densities and electrical conductances of amino acids + ionic liquid ([HMIm]Br) + H2O mixtures at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2010.04.002
Investigation on molecular interaction of amino acids in aqueous disodium hydrogen phosphate solutions with reference to volumetric and compressibility measurements:	https://www.doi.org/10.1016/j.jct.2013.11.015
Volumetric and viscometric properties of amino acids in aqueous maltitol solutions at T = (293.15 to 323.15) K:	https://www.doi.org/10.1016/j.jct.2017.02.024
Viscometric study of glycine, L-alanine, glycylglycine in aqueous tetra-n-alkylammonium bromide solutions at 298.15 K:	https://www.doi.org/10.1016/j.jct.2004.07.006
Thermodynamic modeling of quaternary (CaCl2+Ca(NO3)2+L-alanine+water) system at T = (298.2, 303.2 and 308.2) K: Experimental measurements and thermodynamic modeling:	https://www.doi.org/10.1016/j.fluid.2017.01.014
Volumetric and Viscometric Studies of Amino Acids in Mannitol Aqueous Solutions at T = (298.15 to 318.15) K:	https://www.doi.org/10.1021/je501178z
Water Activity Measurement for Alanine + Dipotassium Oxalate + Water and the Corresponding Binary Solutions at Different Temperatures:	https://www.doi.org/10.1021/je100760v
Effect of concentration and temperature on apparent molar properties of homologous alpha-amino acids in aqueous semicarbazide hydrochloride solutions: A quest on the concept of kosmotropic/chaotropic behaviour of amino acids:	https://www.doi.org/10.1016/j.jct.2019.03.011
Volumetric and viscometric study of amino acids in aqueous sorbitol solutions at different temperatures:	https://www.doi.org/10.1016/j.jct.2015.10.002
Effect of 1-butyl-4-methyl pyridinium iodide, [C4mpy]I, ionic liquid on hydration behaviour of biologically active compounds in aqueous solutions of alpha-amino acids at different temperatures through [illegible]	https://www.doi.org/10.1016/j.jct.2017.08.010
Solvation behaviour of aqueous [illegible] drug at different temperatures: volumetric and ultrasonic study:	https://www.doi.org/10.1016/j.jct.2014.03.015
Volumetric Properties of Glycine, L-Alanine, and L-Serine in Formamide + Water Mixtures at 298.15 K:	https://www.doi.org/10.1021/je5003797
Transfer Partial Molar Volumes of L-Alanine/L-Glutamine/Glycylglycine from Water to 0.512 mol/kg Aqueous KNO3/K2SO4 Solutions at (298.15 to 323.15) K:	https://www.doi.org/10.1021/je300083m
Temperature and concentration dependence towards physicochemical and spectral studies of glycine, L-alanine and L-valine in aqueous solutions of nortriptyline hydrochloride:	https://www.doi.org/10.1016/j.jct.2018.09.026
Physicochemical Behavior of Some Amino Acids/Glycylglycine in Aqueous D-galactose Solutions at Different Temperatures:	https://www.doi.org/10.1007/s10765-010-0742-8
Volumetric and Viscosity Properties of Monosaccharides in Aqueous Amino Acid Solutions at 298.15 K:	https://www.doi.org/10.1021/je050412t
Thermophysical properties of l-Alanine/l-Valine in aqueous solutions of non steroid anti inflammatory drug dolonex at different temperatures: Volumetric and acoustic approach:	https://www.doi.org/10.1016/j.jct.2018.03.022
Interactions 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.2013.08.010
Solvation Behavior of Glycine, L-Alanine, and L-Valine in Aqueous Solutions of Triammonium Citrate at Different Temperatures with Reference to Speeds of Sound Measurements:	https://www.doi.org/10.1007/s10765-015-2006-0
Salting-out effect in polypropylene glycol-amino acid aqueous solutions investigated by vapor pressure osmometry:	https://www.doi.org/10.1016/j.fluid.2016.05.025
Probing solute-solvent interactions of some bio-active solutes inaqueous barium nitrate solution on the basis of physicochemical contrivances:	https://www.doi.org/10.1016/j.tca.2013.06.017
Partial molar volumes of L-alanine, DL-serine, DL-threonine, L-histidine, glycine, and glycylglycine in water, NaCl, and DMSO aqueous solutions at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2005.03.015
Measuring and modeling aqueous electrolyte/amino-acid solutions with ePC-SAFT:	https://www.doi.org/10.1016/j.jct.2013.08.018
Thermodynamics of proton dissociations from aqueous alanine at temperatures from (278.15 to 393.15) K, molalities from (0.0075 to 1.0) mol*kg-1, and at the pressure 0.35 MPa: Apparent molar heat capacities and apparent molar volumes of alanine, alaninium chloride, and sodium alaninate:	https://www.doi.org/10.1016/j.jct.2005.10.007
Effect of KCl and KNO3 on Partial Molal Volumes and Partial Molal Compressibilities of Some Amino Acids at Different Temperatures:	https://www.doi.org/10.1007/s10765-008-0514-x
Interaction of homologous series of amino acids with sarcosine in presence of denaturant: Volumetric and calorimetric approach:	https://www.doi.org/10.1016/j.jct.2013.09.009
Activity Coefficient Measurements and Thermodynamic Modeling of (CaCl2 + l-Alanine + Water) System Based on Potentiometric Determination at T = (298.2, 303.2, and 308.2) K:	https://www.doi.org/10.1021/acs.jced.5b00260
Water Activity in Aqueous Amino Acid Solutions, with and without KCl, at 298.15 K:	https://www.doi.org/10.1021/je700466s
Density and Viscosity Study of Interactions of Some Amino Acids in Aqueous Solutions of Sodium Benzoate:	https://www.doi.org/10.1021/acs.jced.5b01031
Interactions of amino acids and peptides with the drug pentoxifylline in aqueous solution at various temperatures: A volumetric approach:	https://www.doi.org/10.1016/j.jct.2012.05.009
Interaction of some hydrophobic amino acids, peptides, and protein with aqueous 3-chloro-1,2-propanediol and 3-chloro-1-propanol: Biophysical studies:	https://www.doi.org/10.1016/j.jct.2010.11.015
Thermodynamic Study of Some Amino Acids, 2-Aminopropanoic Acid, 2-Amino-3-methylbutanoic Acid, 2-Amino-4-methylpentanoic Acid, and 2-Amino-3-phenylpropanoic Acid in Aqueous Saccharide Solutions at Different Temperatures: Volumetric and Ultrasonic Study:	https://www.doi.org/10.1021/je100857s
Mode of action of betaine on some amino acids and globular proteins: Thermodynamic considerations:	https://www.doi.org/10.1016/j.jct.2017.03.025

Transfer Partial Molar Isentropic Compressibilities of (l-Alanine/l-Glutamine/Glycylglycine) from Water to 0.512 mol*kg-1 Aqueous KNO3/0.512 mol*kg-1 KNO3/0.512 mol*kg-1 Aqueous K2SO4 Solutions Between 298.15 K and 323.15 K:	https://www.doi.org/10.1007/s10765-013-1432-0
Effect of Potassium Citrate Salts on the Transport Behavior of L-Alanine in Aqueous Solutions at T = (293.15 to 308.15) K:	https://www.doi.org/10.1021/je800559d
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C338692&Units=SI
Intermolecular interactions of .alpha.-amino acids and glycyl dipeptides with the drug domiphen bromide in aqueous solutions analyzed by volumetric and UV-vis spectroscopy methods:	https://www.doi.org/10.1016/j.jct.2016.06.018
Interactions in L-alanine / L-proline / L-valine / L-leucine aqueous KCl/KNO3 systems at different temperatures: An isentropic compressibility study:	https://www.doi.org/10.1016/j.tca.2008.10.023
Ternary phase diagram and the formation mechanism of two distinct solid solutions of amino acid systems: L-Valine/L-norvaline and L-valine/L-alanine:	https://www.doi.org/10.1016/j.jct.2017.12.010
Volumetric behaviour of amino acids and their group contributions in aqueous lactose solutions at different temperatures:	https://www.doi.org/10.1016/j.jct.2010.08.004
Vapor pressure osmometry determination of vapor-liquid equilibria behavior of aqueous imidazolium-based ionic liquid + amino acid systems:	https://www.doi.org/10.1016/j.fluid.2017.05.019
Investigation on solute solvent interactions of glycine, L-alanine and L-valine in aqueous tetraethylammonium iodide solutions at different temperatures with reference to volumetric and acoustic measurements:	https://www.doi.org/10.1016/j.jct.2015.08.009
Solute-solvent interactions of glycine, L-alanine and L-valine in aqueous [illegible] solutions at different temperature [illegible] to 308.15) K:	https://www.doi.org/10.1016/j.jct.2015.07.038
Measurement of water activities of alanine + tri-potassium citrate + water system at temperatures between 293.15 and 313 K Experimental and modeling:	https://www.doi.org/10.1016/j.fluid.2008.02.015
Solubility of the Proteinogenic a-Amino Acids in Water, Ethanol, and Ethanol-Water Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00486
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Study of solvation consequences of glycine, L-alanine and L-valine in aqueous 1-butyl-4-methyl pyridinium chloride ionic liquid solutions probed by physicochemical approach in the temperature interval (288.15-308.15) K:	https://www.doi.org/10.1016/j.jct.2017.02.021
Enthalpic interactions between some amino acids and cyclohexanone in aqueous solutions at 298.15 K:	https://www.doi.org/10.1016/j.tca.2006.07.009
Temperature Dependences and Enthalpic Discrimination of Homochiral Pairwise Interactions of Six a-Amino Acid Enantiomers in Pure Water:	https://www.doi.org/10.1021/je500825a
Thermodynamics of (solute + solute) and (solute + solvent) interactions of homologous series of amino acids with thiamine hydrochloride in aqueous medium at T = (305.15, 310.15, 315.15) K: A volumetric and acoustic approach:	https://www.doi.org/10.1016/j.jct.2016.06.026
Infinite Dilution Binary Diffusion Coefficients of Several r-Amino Acids in Water over a Temperature Range from [illegible] K with the Taylor Dispersion Technique:	https://www.doi.org/10.1021/je060149b
Physicochemical Properties of L-Alanine in Aqueous Silver Sulphate Solutions at (298.15, 303.15, 308.15, and 318.15) K:	https://www.doi.org/10.1007/s10765-011-1060-5
Influence of [illegible] Ionic Liquids on the Solubility of l-Alanine and l-Glutamic Acid in Aqueous Solutions at 30 deg C:	https://www.doi.org/10.1021/acs.jced.6b00367
Studies on the Diffusion Coefficients of Amino Acids in Aqueous Solutions:	https://www.doi.org/10.1021/je049582g
Apparent Molar Volumes and Viscosity B-Coefficients of Some Amino Acids in Aqueous Tetramethylammonium Iodide Solutions at 298.15 K:	https://www.doi.org/10.1021/je7001418
Solute-solvent interactions of glycine, L-alanine, and L-valine in aqueous 1-methyl-3-octylimidazolium chloride ionic liquid solutions in the temperature interval (288.15-308.15) K:	https://www.doi.org/10.1016/j.tca.2014.06.028
Volumetric and viscometric studies of amino acids in L-ascorbic acid aqueous solutions at T = (293.15 to 323.15) K:	https://www.doi.org/10.1016/j.jct.2013.11.002
Enthalpies of dilution of glycine, L-alanine and L-serine in aqueous potassium chloride solutions:	https://www.doi.org/10.1016/j.tca.2004.05.021
Study of (solute + solute) and (solute + solvent) interactions of homologous series of some .alpha.-amino acids in aqueous streptomycin sulfate solutions at different temperatures by physicochemical methods:	https://www.doi.org/10.1016/j.jct.2015.11.015
Study of solvation consequences of alpha amino acids in aqueous [illegible] probed by [illegible] approach:	https://www.doi.org/10.1016/j.fluid.2013.03.030
Study of solute-solute and solute-solvent interactions of homologous series of some .alpha.-amino acids in aqueous D-xylose solutions at different temperatures by using physicochemical methods:	https://www.doi.org/10.1016/j.jct.2016.06.030
Densities and viscosities of amino acid + xylitol + water solutions at 293.15 to 323.15 K:	https://www.doi.org/10.1021/acs.jced.6b00766
Interactions of some amino acids and glycine peptideswith aqueous sodium dodecyl sulfate and cetyltrimethylammonium bromide at T = 298.15 K: a volumetric approach:	https://www.doi.org/10.1016/j.jct.2003.09.010
Volumetric property of glycine, L-serine, L-alanine and L-proline in aqueous solutions of 1-phenylpiperazinium [illegible] an active pharmaceutical ingredient ionic liquid (API-IL) in the aqueous amino acids solutions:	https://www.doi.org/10.1016/j.jct.2016.03.045
Conductometric analysis of 1-butyl-3-methylimidazolium tetrafluoroborate:	https://www.doi.org/10.1016/j.jct.2016.07.047
Volumetric properties of L-alanine, and L-valine in aqueous sucrose solutions at T = (288.15 to 323.15) K:	https://www.doi.org/10.1016/j.jct.2004.12.015
Thermodynamics of the ternary systems: (water + glycine, L-alanine and L-serine + di-ammonium hydrogen citrate) from volumetric, compressibility, and (vapour + liquid) equilibria measurements:	https://www.doi.org/10.1016/j.jct.2010.08.021
Solvation behavior of some amino acids in aqueous solutions of [illegible] drug at different temperatures analysed by volumetric and acoustic methods:	https://www.doi.org/10.1016/j.jct.2016.03.016
Densities and Speeds of Sound of Glycine, L-Alanine, and L-Valine in Aqueous [illegible] Chloride Solutions at Different Temperatures:	https://www.doi.org/10.1021/je500324a
Low-temperature heat capacities and standard molar enthalpy of formation of the solid-state coordination compound trans-Cu(Ala)2(s) (Ala = L-alanine):	https://www.doi.org/10.1016/j.tca.2008.02.024
Viscosity studies of L-alanine, L-proline, L-valine, L-leucine + aqueous KCl/KNO3) solutions at different temperatures:	https://www.doi.org/10.1016/j.jct.2008.07.019
Densities and Speeds of Sound of Solutions of Glycine, l-Alanine, and l-Valine in Aqueous Ammonium Dihydrogen Phosphate at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.7b00257
Study of Solvation Behavior of Some Biologically Active Compounds in Aqueous Barium Chloride Solution:	https://www.doi.org/10.1021/je400077c
Densities, Viscosities, Electrical Conductances, and Refractive Indices of Amino Acid + Ionic Liquid ([BMIm]Br) + Water Mixtures at 298.15 K:	https://www.doi.org/10.1021/je900882r
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Interactions in (L-alanine / L-threonine + aqueous glucose / aqueous sucrose) systems at 298.15- 323.15 K:	https://www.doi.org/10.1016/j.tca.2011.10.013

Enthalpies of Dilution of l-Alanine in Dimethylsulfoxide + Water and Dimethylformamide + Water Mixtures at 298.15 K: https://www.doi.org/10.1021/je9005322

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
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume