L-Valine

Other names:	(S)-(+)-valine (S)-2-Amino-3-methylbutanoic acid (S)-2-Amino-3-methylbutyric acid (S)-3-amino-2-methylbutanoic acid (S)-Valine 2-Amino-3-methylbutanoic acid 2-Amino-3-methylbutyric acid Butanoic acid, 2-amino-3-methyl- L-(+)-«alpha»-Aminoisovaleric acid L-2-amino-3-methylbutanoic acid L-2-amino-3-methylbutyric acid L-2-aminoisovaleric acid L-iso-C3H7CH(NH2)COOH NSC 76038 Valine, L- butanoic acid, 2-amino-3-methyl-, (S)- Valine
Inchi:	InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1
InchiKey:	KZSNJWFQEVHDMF-BYPYZUCNSA-N
Formula:	C5H11NO2
SMILES:	CC(C)[C@H](N)C(=O)O
Mol. weight [g/mol]:	117.15
CAS:	72-18-4

Physical Properties

Property code	Value	Unit	Source
af	0.6240		Cheméo Relay (1.0)
affp	910.60	kJ/mol	NIST Webbook
basg	876.70	kJ/mol	NIST Webbook
basg	873.00 ± 3.00	kJ/mol	NIST Webbook
chs	-2910.70 ± 1.90	kJ/mol	NIST Webbook
chs	-2920.10 ± 0.54	kJ/mol	NIST Webbook
hf	-477.12	kJ/mol	Cheméo Relay (1.0)
hfs	-618.00	kJ/mol	NIST Webbook
hfs	-628.90 ± 1.90	kJ/mol	NIST Webbook
hfus	17.00	kJ/mol	Joback Method
hvap	66.04	kJ/mol	Cheméo Relay (1.0)

ie	8.71	eV	NIST Webbook
log10ws	-0.31		Aqueous Solubility Prediction Method
logp	0.054		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	4238.55	kPa	Joback Method
ss	178.87	J/mol×K	NIST Webbook
tb	475.95	K	Cheméo Relay (1.0)
tc	661.75	K	Cheméo Relay (1.0)
tf	588.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
tf	585.65	K	Aqueous Solubility Prediction Method
vc	0.349	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	168.50	J/mol×K	298.15	NIST Webbook
cps	168.82	J/mol×K	298.15	NIST Webbook
hsubt	163.00 ± 0.80	kJ/mol	455.00	NIST Webbook
hsubt	163.00 ± 8.00	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	6.07000e+00
Coeff. B	6.03340e-01
Coeff. C	-3.70600e-04
Coeff. D	8.63000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Surface Tension of Aqueous Solutions of Small-Chain Amino and Organic Acids:	https://www.doi.org/10.1021/acs.jced.9b00026
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
Densities, Viscosities, Electrical Conductances, and Refractive Indices of Amino Acid + Ionic Liquid (BMIMBr) + Water Mixtures at 298.15 K: Measurement and Correlation:	https://www.doi.org/10.1021/je900882r
Partial molar volume and partial molar compressibility of four homologous amino acids in aqueous sodium bromide solutions at different temperatures:	https://www.doi.org/10.1016/j.jct.2011.01.004
Solubility of L-valine in Water, Ethanol, Acetone, and Acetonitrile at 278.15 to 318.15 K:	https://www.doi.org/10.1021/je500035r
Solute–solvent interactions of glycine, L-alanine, and L-valine in aqueous 1-ethyl-3-methylimidazolium chloride ionic liquid solutions at the temperature interval 298.15 to 318.15 K:	https://www.doi.org/10.1016/j.jct.2015.07.038
Isopiestic Activity Coefficients and Excess Gibbs Energies of Aqueous 1-Ethyl-3-methylimidazolium Chloride Ionic Liquid at 298.15 K:	https://www.doi.org/10.1021/je060149b
Thermodynamic properties of aqueous solutions of alpha-amino acids at different temperatures through conductometric and ultrasonic studies:	https://www.doi.org/10.1016/j.jct.2017.08.010
Activity coefficients of glycine, d-alanine and l-valine in aqueous solutions containing MgSO4 at 298.15 K:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Experimental Determination and Correlation of Densities of Aqueous Amino Acids in Mannitol Aqueous Solutions at T = (298.15 to 323.15) K:	https://www.doi.org/10.1016/j.fluid.2011.10.015
Thermochemistry of glycine·2.15Ca(NO3)2·10H2O(s) by a calorimetrical approach in the (A = L-valine and methionine):	https://www.doi.org/10.1016/j.jct.2017.02.021
Densities and Speeds of Sound of Glycine, l-Alanine, and l-Valine in Aqueous 1-Ethyl-3-methylimidazolium Chloride Solutions at Different Temperatures:	https://www.doi.org/10.1021/je501178z
Interactions of glycine, L-alanine and L-valine with aqueous solutions of tetrabutylammonium bromide at different temperatures: A volumetric and viscometric approach:	https://www.doi.org/10.1016/j.tca.2005.04.031
Volumetric and viscometric studies of amino acids in aqueous sorbitol solutions at 298.15 K:	https://www.doi.org/10.1021/je500324a
Enthalpic interactions between some amino acids and cyclohexanone in aqueous solutions at 298.15K:	https://www.doi.org/10.1016/j.jct.2013.08.010
Interactions of some amino acids and glycine peptideswith aqueous sodium bromide solutions at 298.15K:	https://www.doi.org/10.1016/j.jct.2013.11.002
Effect of concentration and temperature on apparent molar volume of tetrabutyl ammonium bromide at T = (298.15 to 328.15) K: a volumetric approach:	https://www.doi.org/10.1021/je7006082
Study of thermodynamic properties of amino acids in aqueous solutions of 2-amino-1-propanol hydrochloride solutions: A decision on the hydrophobic–hydrophilic balance of amino acids:	https://www.doi.org/10.1016/j.jct.2015.10.002
Thermodynamics of the interactions of a homologous series of some amino acids in aqueous solutions of 2-Amino-1-propanol at 298.15 K:	https://www.doi.org/10.1016/j.tca.2006.07.009
Volumetric, compressibility, and viscometric studies of some hydrophobic amino acids, peptides, and protein with aqueous solutions of 2-Amino-1-propanol at 298.15K:	https://www.doi.org/10.1016/j.jct.2003.09.010
Solute–solvent interactions of glycine, L-alanine, and L-valine in aqueous 1-methyl-3-octylimidazolium chloride ionic liquid solutions at the temperature interval (288.15 to 318.15) K and at Atmospheric Pressure:	https://www.doi.org/10.1016/j.jct.2019.03.011
Interaction of homologous series of amino acids with sucrose in presence of antibacterial drug Chemeo Relavl (D_beta):	https://www.doi.org/10.1016/j.jct.2012.12.010
Volumetric and Viscometric Studies of Some Amino Acids in Aqueous Solution at Different Temperatures:	https://www.doi.org/10.1016/j.jct.2011.05.012
Thermodynamic Study of the Interactions of Some Amino Acids with Tetrabutylammonium Bromide in Aqueous Solutions at 298.15 K:	https://www.doi.org/10.1016/j.tca.2008.09.001
Volumetric and viscometric studies of natural amino acids in aqueous solutions:	https://www.doi.org/10.1016/j.jct.2010.11.015
Study of the interactions of glycine, L-alanine, and L-valine in aqueous solutions of 1-Ethyl-3-methylimidazolium Chloride Ionic Liquid at Different Temperatures:	https://www.doi.org/10.1016/j.jct.2013.10.022
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 to 318.15) K and at Atmospheric Pressure:	https://www.doi.org/10.1016/j.tca.2014.06.028
Volumetric and Viscometric Studies of Some Amino Acids in Aqueous Solution at Different Temperatures:	https://www.doi.org/10.1021/je100909b
Solution behaviour of biologically active compounds in aqueous amino acids solutions at different temperatures:	https://www.doi.org/10.1016/j.jct.2014.03.015
Interaction of homologous series of amino acids with sucrose in presence of denaturant: Volumetric and calorimetric approach:	https://www.doi.org/10.1016/j.jct.2013.09.009
Transfer Enthalpies of Amino Acids and Glycine Peptides from Water to Aqueous Solutions of Trimethylamine N-Oxide at 298.15 K:	https://www.doi.org/10.1016/j.tca.2014.04.013
Intermolecular interactions of alpha-amino acids and glycyl dipeptides with the drug pentoxifylline in aqueous solution at various temperatures: A volumetric approach:	https://www.doi.org/10.1016/j.jct.2016.06.018
Molecular interactions between some amino acids and a pharmaceutically active drug in aqueous solutions analyzed by volumetric and UV–Vis spectroscopy methods:	https://www.doi.org/10.1016/j.jct.2019.06.002
Interactions in L-alanine/L-proline + divalent leucine aqueous cinnamate systems at various temperatures:	https://www.doi.org/10.1016/j.tca.2008.10.023
Solution Behavior of Some Biologically Active Compounds in Aqueous Barium Chloride Solution:	https://www.doi.org/10.1021/je400077c
Isentropic compressibility study:	https://www.doi.org/10.1016/j.jct.2012.05.009

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
Thermodynamics of solution of Leucine in water:	https://www.doi.org/10.1016/j.tca.2017.10.020
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72184&Units=SI
Investigations on molecular interaction of some amino acids with the drug levofloxacin in aqueous solution by	https://www.doi.org/10.1016/j.jct.2016.09.027
Densities and Speeds of Sound of Solutions of Glycine, L-Alanine, and L-Valine in Aqueous Potassium Dihydrogen Phosphate at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.7b00257
Acoustic and Thermodynamic Studies of Some Amino Acids in Aqueous Solutions of Ethanol at different Temperatures:	https://www.doi.org/10.1021/je100857s
Study of solute (amino acid) + solvent) interactions of homologous	https://www.doi.org/10.1016/j.jct.2015.11.015
Volumetric and viscometric properties of some amino acids in aqueous solutions of	https://www.doi.org/10.1016/j.jct.2017.02.024
Solubility of Amino Acids in Different Solvent Mixtures	https://www.doi.org/10.1016/j.jct.2018.09.026
Solubility of Amino Acids in Water: Determination of solubility dependence	https://www.doi.org/10.1016/j.tca.2013.06.017
Solubility of some amino acids in water and pH dependence of the solubility	https://www.doi.org/10.1021/je049582g
Estimation of Aqueous Solubility of Amino Acids:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Effect of hydrophilic additives on volumetric and viscosity properties of amino acids in aqueous solutions at	https://www.doi.org/10.1016/j.jct.2011.12.020
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
Thermodynamic properties of alanine, and L-valine in aqueous sucrose solutions at T = (288.15 and 308.15) K:	https://www.doi.org/10.1016/j.jct.2017.03.025
Investigation on molecular interaction of amino acids in aqueous disodium hydrogen phosphate solutions with	https://www.doi.org/10.1016/j.jct.2004.12.015
Volumetric, ultrasonic, and viscometric behaviour of glycine, DL-alanine, and L-valine in aqueous solutions at different temperatures:	https://www.doi.org/10.1016/j.jct.2013.11.015
Jean-Claude Bradley Open Melting Point Dataset (2017-GCC6):	https://www.doi.org/10.1016/j.jct.2008.09.008
Thermodynamic measurements of Solvation Behavior of Glycine,	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
l-Alanine, and l-Valine in Aqueous Solutions at Different Temperatures:	https://www.doi.org/10.1007/s10765-015-2006-0
Viscosity studies of d-alanine, DL-alanine, L-leucine, L-valine in aqueous solutions of Trisodium Citrate at different temperatures:	https://www.doi.org/10.1016/j.jct.2008.07.019
Study of solute-solute and solute-solvent interactions of homologous series of some alpha-amino acids in aqueous solutions of	https://www.doi.org/10.1016/j.jct.2016.06.030
Densities, Sound Speed, and Viscosities of Some Amino Acids with Aqueous Benzamide at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.5b00198
Volumetric behaviour of amino acids and their group contributions in aqueous sodium bromide solutions at different temperatures:	https://www.doi.org/10.1016/j.jct.2010.08.004
Thermophysical properties of physicochemical methods.	https://www.doi.org/10.1016/j.jct.2018.03.022
Solubility of glycine at different temperature in aqueous solutions of non steroid anti inflammatory drug dolonex at different temperatures:	http://link.springer.com/article/10.1007/BF02311772
McGowan Method:	
Solvation behavior of some amino acids in aqueous solutions of non steroidal anti inflammatory drug sodium diclofenac at different temperatures analysed by volumetric and acoustic methods.	https://www.doi.org/10.1016/j.jct.2016.03.016
Measuring and modeling aqueous electrolyte/amino acid solutions with	https://www.doi.org/10.1016/j.jct.2013.08.018
Aqueous phase diagram and the formation mechanism of two distinct solid solutions of amino acid systems.	https://www.doi.org/10.1016/j.jct.2017.12.010
Volumetric and Viscometric Studies of Amino Acids in Vitamin B6 Aqueous Solutions at Different Temperatures:	https://www.doi.org/10.1021/je500975a
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
Measurement and Correlation of Solubility of l-Valine in Water + (Ethanol, 1,4-Dimethylbenzene, Acetone, Isopropyl Alcohol) from 293.15 K to 343.15 K:	https://www.doi.org/10.1021/je500255d
Study of solvation consequences of alpha-amino acids in aqueous	https://www.doi.org/10.1016/j.fluid.2013.03.030
Physicochemical study of solute-solute and solute-solvent interactions of	https://www.doi.org/10.1016/j.jct.2016.03.012
Investigation of Volumetric and Acoustic Properties of Procainamide Hydrochloride in Aqueous-D-mannose Solutions at Temperatures from 298.15	https://www.doi.org/10.1021/acs.jced.7b00452
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Densities and viscosities of amino acid + xylitol + water solutions at 293.15	https://www.doi.org/10.1021/acs.jced.6b00766
Investigation on solute solvent interactions of glycine, L-alanine and L-valine in aqueous	https://www.doi.org/10.1016/j.jct.2015.08.009
Thermodynamics of (solute + solute) and (solute + solvent) interactions of	https://www.doi.org/10.1016/j.jct.2016.06.026
Structural Interactions between Amino Acids and Zinc Chloride in Aqueous Solutions at Different Temperatures:	https://www.doi.org/10.1021/je8001464
Thermochemical and Acoustic Studies of Glycine and L-Valine in Aqueous Solutions at T = (298.15, 308.15, 318.15) K: A Volumetric and Acoustic Approach:	https://www.doi.org/10.1021/je400894j
Measurement and Correlation of Solubility of Amino Acids in Aqueous Trisodium Citrate Solutions at Different Temperatures:	

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
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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