(-)-D-arginine hydrate

Other names: D-Arginine
L-arginine
Inchi: InChI=1S/C6H14N4O2/c7-4(5(11)12)2-1-3-10-6(8)9/h4H,1-3,7H2,(H,11,12)(H4,8,9,10)/t4
InchiKey: ODKSFYDXXFIFQN-BYPYZUCNSA-N
Formula: C6H14N4O2
SMILES: N=C(N)NCCCC(N)C(=O)O
Mol. weight [g/mol]: 174.20
CAS: 157-06-2

Physical Properties

Property code	Value	Unit	Source
chs	-3738.30 ± 1.30	kJ/mol	NIST Webbook
gf	157.35	kJ/mol	Joback Method
hf	-117.88	kJ/mol	Joback Method
hfs	-623.60 ± 1.30	kJ/mol	NIST Webbook
hvap	91.79	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	-1.338		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
ss	250.60	J/mol×K	NIST Webbook
tb	761.86	K	Joback Method
tf	541.09	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.74	J/mol×K	761.86	Joback Method
cpg	82.60	J/mol×K	100.12	Joback Method
cpg	82.60	J/mol×K	100.12	Joback Method
cpg	82.60	J/mol×K	100.12	Joback Method
cpg	82.60	J/mol×K	100.12	Joback Method
cpg	82.60	J/mol×K	100.12	Joback Method
cpg	82.60	J/mol×K	100.12	Joback Method
cps	232.80	J/mol×K	296.80	NIST Webbook

Sources

Partial molar volumes and viscosity B-coefficients of arginine in aqueous glucose, sucrose and L-ascorbic acid solutions at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2004.07.030
Volumetric, acoustic and transport properties of ternary solutions of L-serine and L-arginine in aqueous solutions of thiamine hydrochloride at different temperatures:	https://www.doi.org/10.1016/j.jct.2019.03.039
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination and Correlation of the Solubility of l-Fucose in Four Binary Solvent Systems at the Temperature Range from 283.15 to 308.15 K:	https://www.doi.org/10.1021/acs.jced.8b00361
Volumetric and Viscometric Studies of Amino Acids in Vitamin B6 Aqueous solutions at Various Temperatures:	https://www.doi.org/10.1021/je500975a
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Volumetric and Viscometric Studies of Amino Acids in Mannitol Aqueous Solutions at T = (293.15 to 323.15) K:	https://www.doi.org/10.1021/je501178z
Solubility of the Proteinogenic α-Amino Acids in Water, Ethanol, and Ethanol–Water Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00486
Volumetric and viscometric study of amino acids in aqueous sorbitol solution at different temperatures:	https://www.doi.org/10.1016/j.jct.2015.10.002
Study of thermodynamic properties of aqueous binary mixtures of L-threonine, L-valine and L-arginine at T = (293.15 to 323.15) K:	https://www.doi.org/10.1016/j.jct.2012.12.010
Densities and viscosities of amino acid + xylitol + water solution at 293.15 and 298.15 K:	https://www.doi.org/10.1021/acs.jced.6b00766
NIST Webbook (for T > 323.15):	http://webbook.nist.gov/cgi/cbook.cgi?ID=C157062&Units=SI
Volumetric Behavior on Interactions of a-Amino Acids with Sodium Acetate, Potassium Acetate, and Calcium Acetate in Aqueous Solutions:	https://www.doi.org/10.1021/je100190e
Predicting solute-solute and solute-solvent interactions in (L-arginine + d-xylose/l-arabinose + water) solutions at different temperatures by using volumetric and viscometric methods:	https://www.doi.org/10.1016/j.jct.2013.04.001
Volumetric and viscometric properties of amino acids in aqueous maltitol solutions at different temperatures:	https://www.doi.org/10.1016/j.jct.2017.02.024
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
Viscosity Behavior of alpha-Amino Acids in Acetate Salt Solutions at Temperatures (303.15 to 323.15) K:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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/10.1007/s10765-011-1111-y
McGowan Method:	https://www.doi.org/10.1016/j.jct.2013.11.002
Studies on the Diffusion Coefficients of Amino Acids in Aqueous Solutions:	http://link.springer.com/article/10.1007/BF02311772
	https://www.doi.org/10.1021/je049582g

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
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
ss:	Solid phase molar entropy at standard conditions

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point