L-Asparagine

Other names:	(-)-Asparagine
	(S)-2,4-Diamino-4-oxobutanoic acid
	(S)-Asparagine
	Agedoite
	Altheine
	Asn
	Asparagine
	Asparagine acid
	Asparagine l(-)
	Asparagine, L-
	Asparamide
	Aspartamic acid
	Aspartic acid «beta» amide
	Aspartic acid Â«betaÂ» amide
	Butanoic acid, 2,4-diamino-4-oxo-, (S)-
	Crystal VI
	L-2,4-Diamino-4-oxobutanoic acid
	L-asparagine (anhydrous)
	L-«beta»-Asparagine
	L-Â«betaÂ»-Asparagine
	NSC 82391
	«alpha»-Aminosuccinamic acid
	Â«alphaÂ»-Aminosuccinamic acid
Inchi:	InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m1/s1
InchiKey:	DCXYFEDJOCDNAF-UWTATZPHSA-N
Formula:	C4H8N2O3
SMILES:	NC(=O)CC(N)C(=O)O
Mol. weight [g/mol]:	132.12
CAS:	70-47-3

Physical Properties

Property code	Value	Unit	Source
affp	929.00	kJ/mol	NIST Webbook
affp	937.60	kJ/mol	NIST Webbook
affp	965.20 ± 5.20	kJ/mol	NIST Webbook
basg	891.50	kJ/mol	NIST Webbook

basg	920.00 ± 5.60	kJ/mol	NIST Webbook
chs	-1928.50 ± 0.71	kJ/mol	NIST Webbook
ep	-43.00 ± 7.00	J/mol×K	NIST Webbook
gf	-281.40	kJ/mol	Joback Method
hf	-440.98	kJ/mol	Joback Method
hfs	-789.02	kJ/mol	NIST Webbook
hfus	112.48	kJ/mol	THE STANDARD ENTHALPIES OF FORMATION OF L-ASPARAGINE AND L-a-GLUTAMINE
hvap	75.56	kJ/mol	Joback Method
log10ws	-0.83		Aqueous Solubility Prediction Method
logp	-1.726		Crippen Method
mcvol	96.190	ml/mol	McGowan Method
pc	6278.87	kPa	Joback Method
ss	174.50	J/mol×K	NIST Webbook
tb	635.46	K	Joback Method
tc	841.61	K	Joback Method
tf	507.65	K	Aqueous Solubility Prediction Method
vc	0.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.85	J/mol×K	635.46	Joback Method
cpg	250.50	J/mol×K	669.82	Joback Method
cpg	256.73	J/mol×K	704.18	Joback Method
cpg	262.56	J/mol×K	738.53	Joback Method
cpg	268.00	J/mol×K	772.89	Joback Method
cpg	273.05	J/mol×K	807.25	Joback Method
cpg	277.73	J/mol×K	841.61	Joback Method
cps	159.80	J/mol×K	296.50	NIST Webbook

Sources

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

Intermolecular/interionic interactions in l-leucine-, l-asparagine-, and glycylglycine aqueous electrolyte systems:	https://www.doi.org/10.1016/j.tca.2006.04.004
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Study of the interactions of PAMAM-NH2 G4 dendrimer with selected natural amino acids in aqueous solutions:	https://www.doi.org/10.1016/j.jct.2013.10.022
Effect of hydrophilic additives on volumetric and viscosity properties of amino acids in aqueous solutions at T = (293.15 to 323.15) K:	https://www.doi.org/10.1016/j.jct.2011.12.020
Physicochemical study of (solute + solute) and (solute + solvent) interactions of L-asparagine and L-glutamine in aqueous-D-mannose solutions at temperatures from (293.15 to 318.15) K:	https://www.doi.org/10.1016/j.jct.2015.11.014
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70473&Units=SI
THE STANDARD ENTHALPIES OF FORMATION OF L-ASPARAGINE AND L-α-GLUTAMINE:	https://www.doi.org/10.1016/j.tca.2009.08.017
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
ep:	Protonation entropy at 298K
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