L-Asparagine, hydrate (1:1)

Other names:	L-Asparagine Monohydrate
Inchi:	InChI=1S/C4H8N2O3.H2O/c5-2(4(8)9)1-3(6)7;/h2H,1,5H2,(H2,6,7)(H,8,9);1H2/t2-;/m1./s
InchiKey:	RBMGJIZCEWRQES-HSHFZTNMSA-N
Formula:	C4H10N2O4
SMILES:	NC(=O)CC(N)C(=O)O.O
Mol. weight [g/mol]:	150.13
CAS:	5794-13-8

Physical Properties

Property code	Value	Unit	Source
chs	-1916.60 ± 0.79	kJ/mol	NIST Webbook
chs	-1924.70	kJ/mol	NIST Webbook
hfs	-1086.60 ± 0.84	kJ/mol	NIST Webbook
hfus	135.03	kJ/mol	Solubility of L-asparagine monohydrate in water and water-isopropanol mixed solvents: Measurements and thermodynamic modelling
ss	209.62	J/mol×K	NIST Webbook
ss	213.40	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	207.90	J/mol×K	298.15	NIST Webbook
cps	205.90	J/mol×K	296.70	NIST Webbook

Sources

Solubility of L-asparagine monohydrate in water and water-isopropanol mixed solvents: Measurements and thermodynamic modelling:	https://www.doi.org/10.1016/j.fluid.2015.12.040
THE STANDARD ENTHALPIES OF FORMATION OF L-ASPARAGINE AND L-GLUTAMINE:	https://www.doi.org/10.1016/j.tca.2009.08.017
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5794138&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ss:	Solid phase molar entropy at standard conditions

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