Aspartic acid

Other names:	(2S)-Aspartic acid
	(S)-Aminobutanedioic acid
	(S)-Aspartic acid
	Aminosuccinic acid
	Asparagic acid
	Asparaginic acid
	Aspartic acid, L-
	Aspatofort
	Butanedioic acid, amino-, (S)-
	H-Asp-OH
	L-(+)-Aspartic acid
	L-2-Aminobutanedioic acid
	L-Aminosuccinic acid
	L-Asparagic acid
	L-Asparaginic acid
	L-Aspartic acid
	NSC 3973
	«alpha»-Aminosuccinic acid, (L)-
	Â«alphaÂ»-Aminosuccinic acid, (L)-
Inchi:	InChI=1S/C4H7NO4/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H,6,7)(H,8,9)/t2-/m1/s1
InchiKey:	CKLJMWTZIZZHCS-UWTATZPHSA-N
Formula:	C4H7NO4
SMILES:	NC(CC(=O)O)C(=O)O
Mol. weight [g/mol]:	133.10
CAS:	56-84-8

Physical Properties

Property code	Value	Unit	Source
affp	908.90	kJ/mol	NIST Webbook
basg	875.00	kJ/mol	NIST Webbook
chs	-1617.80	kJ/mol	NIST Webbook
chs	-1601.10 ± 0.79	kJ/mol	NIST Webbook
chs	-1615.60	kJ/mol	NIST Webbook
chs	-1604.40	kJ/mol	NIST Webbook
gf	-484.67	kJ/mol	Joback Method
hf	-627.00	kJ/mol	Joback Method
hfs	-973.32 ± 0.84	kJ/mol	NIST Webbook

hfus	19.16	kJ/mol	Joback Method
hvap	81.60	kJ/mol	Joback Method
log10ws	-1.31		Aqueous Solubility Prediction Method
logp	-1.127		Crippen Method
mcvol	92.080	ml/mol	McGowan Method
pc	6642.18	kPa	Joback Method
ss	173.60	J/mol×K	NIST Webbook
ss	170.12	J/mol×K	NIST Webbook
tb	655.11	K	Joback Method
tc	842.78	K	Joback Method
tf	546.48	K	Aqueous Solubility Prediction Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.47	J/mol×K	655.11	Joback Method
cpg	238.94	J/mol×K	686.39	Joback Method
cpg	244.10	J/mol×K	717.67	Joback Method
cpg	248.94	J/mol×K	748.94	Joback Method
cpg	253.48	J/mol×K	780.22	Joback Method
cpg	257.73	J/mol×K	811.50	Joback Method
cpg	261.69	J/mol×K	842.78	Joback Method
cps	155.18	J/mol×K	298.15	NIST Webbook
cps	152.70	J/mol×K	293.90	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56848&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
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