L-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-Asparagic acid
	L-Asparaginic acid
	L-aminosuccinic acid
	NSC 3973
	«alpha»-Aminosuccinic acid, (L)-
	Aspartic acid
Inchi:	InChI=1S/C4H7NO4/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H,6,7)(H,8,9)/t2-/m0/s1
InchiKey:	CKLJMWTZIZZHCS-REOHCLBHSA-N
Formula:	C4H7NO4
SMILES:	N[C@@H](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	-1601.10 ± 0.79	kJ/mol	NIST Webbook
chs	-1604.40	kJ/mol	NIST Webbook
chs	-1617.80	kJ/mol	NIST Webbook
chs	-1615.60	kJ/mol	NIST Webbook
hf	-771.54	kJ/mol	Cheméo Relay (1.0)
hfs	-973.32 ± 0.84	kJ/mol	NIST Webbook
hfus	28.08	kJ/mol	Joback Method
hvap	93.14	kJ/mol	Cheméo Relay (1.0)

ie	9.23	eV	Cheméo Relay (1.0)
log10ws	-1.31		Aqueous Solubility Prediction Method
logp	-1.127		Crippen Method
mcvol	92.080	ml/mol	McGowan Method
pc	5414.53	kPa	Joback Method
ss	170.12	J/mol×K	NIST Webbook
ss	173.60	J/mol×K	NIST Webbook
tb	528.70	K	Cheméo Relay (1.0)
tc	765.51	K	Cheméo Relay (1.0)
tf	546.48	K	Aqueous Solubility Prediction Method
tf	503.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	155.18	J/mol×K	298.15	NIST Webbook
cps	152.70	J/mol×K	293.90	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	1.32610e+01
Coeff. B	5.53200e-01
Coeff. C	-3.85600e-04
Coeff. D	1.02900e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Thermodynamics of the first and second proton dissociations from aqueous L-aspartic acid and L-glutamic acid at temperatures from (278.15 to 393.15) K and at the pressure 0.35 MPa:	https://www.doi.org/10.1016/j.jct.2006.08.008
Chemeo Relay (1.0):	
Chemeo Relay (1.0_beta):	
Apparent molar heat capacities and apparent molar volumes of zwitterionic, protonated cationic, and deprotonated anionic forms of glycine from (0.002 to 1.00) mol·kg⁻¹ and T = (278.15 to 393.15) K:	https://www.doi.org/10.1021/je100756z
Enthalpic Interaction Coefficients of Several L-α-Amino Acids in Aqueous Solutions from (298 to 343) K:	https://www.doi.org/10.1021/je9007102
Solubility Modeling of L-Aspartic Acid in Aqueous Salt Solutions from (293.15 to 343) K:	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56848&Units=SI
Solubilities of magnesium-L-ascorbate, calcium-L-ascorbate, magnesium-L-glutamate, magnesium-D-gluconate, calcium-D-gluconate, calcium-D-heptagluconate, L-aspartic acid, and 3-nitrobenzoic acid in water:	https://www.doi.org/10.1016/j.jct.2007.12.006
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Modeling solubility and acid-base properties of some polar side chain amino acids in NaCl and (CH3)4NCl aqueous solutions at different ionic strengths and temperatures:	https://www.doi.org/10.1016/j.fluid.2017.11.030
Solubility of the Proteinogenic α-Amino Acids in Water, Ethanol, and Aqueous Ethanol Solutions at Several Temperatures:	https://www.doi.org/10.1021/acs.jced.7b00486
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
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

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