

D-Aspartic acid

Other names:	(-)-Aspartic acid (R)-aspartic acid Asp Aspartic acid D-form D-(-)-Aspartic acid D-aminosuccinic acid L-aminosuccinic acid L-aspartic acid NSC 97922
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:	CKLJMWZTZZHCS-REOHCLBHSA-N
Formula:	C4H7NO4
SMILES:	NC(CC(=O)O)C(=O)O
Mol. weight [g/mol]:	133.10
CAS:	1783-96-6

Physical Properties

Property code	Value	Unit	Source
affp	916.30	kJ/mol	NIST Webbook
gf	-484.67	kJ/mol	Joback Method
hf	-627.00	kJ/mol	Joback Method
hfus	19.16	kJ/mol	Joback Method
hvap	81.60	kJ/mol	Joback Method
log10ws	0.76		Crippen Method
logp	-1.127		Crippen Method
mcvol	92.080	ml/mol	McGowan Method
pc	6642.18	kPa	Joback Method
tb	655.11	K	Joback Method
tc	842.78	K	Joback Method
tf	424.60	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.47	J/molxK	655.11	Joback Method
cpg	238.94	J/molxK	686.39	Joback Method
cpg	244.10	J/molxK	717.67	Joback Method
cpg	248.94	J/molxK	748.94	Joback Method
cpg	253.48	J/molxK	780.22	Joback Method
cpg	257.73	J/molxK	811.50	Joback Method
cpg	261.69	J/molxK	842.78	Joback Method

Sources

Modeling solubility and acid-base properties of some polar side chain amino acids and (CH₃)₄NCI in water: a thermodynamic approach. <https://www.doi.org/10.1016/j.fluid.2017.11.030>

Solubility modeling and thermodynamic properties of different mixtures of N-methyl-2-pyrrolidone, N,N-dimethylformamide, dimethyl sulfoxide and 1,4-dioxane. <https://www.doi.org/10.1016/j.jct.2019.06.025>

Solubility of d-Aspartic Acid and l-Aspartic Acid in Aqueous Salt Solutions from (293 to 343) K: https://www.chemeo.com/doc/models/crippen_log10ws

Crippen Method:

Thermodynamics of the first and second proton dissociations from d-Aspartic Acid and l-Aspartic Acid in Several Neutral Solvents. Determination of Solubility and the Pressure of Amino Acids in Water. Ethanol capacities and apparent molar volumes of zwitterionic, protonated cationic, and deprotonated anionic species of aspartate, glutamate, and glutamate, magnesium-D-gluconate, calcium-D-gluconate, calcium-D-fructogluconate, L-aspartic acid, and 3-nitrobenzoic acid in water: https://en.wikipedia.org/wiki/Joback_method

<https://www.doi.org/10.1021/je9007102>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1783966&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

<https://www.doi.org/10.1016/j.jct.2006.08.008>

<https://www.doi.org/10.1021/acs.jced.9b00320>

<https://www.doi.org/10.1021/acs.jced.7b00486>

<http://link.springer.com/article/10.1007/BF02311772>

<https://www.doi.org/10.1016/j.jct.2007.12.006>

Legend

- affp: Proton affinity
- cpg: Ideal gas heat capacity
- gf: Standard Gibbs free energy of formation
- hf: Enthalpy of formation at standard conditions
- hfus: Enthalpy of fusion at standard conditions
- hvp: Enthalpy of vaporization at standard conditions
- log10ws: Log10 of Water solubility in mol/l
- logp: Octanol/Water partition coefficient
- mcpv: McGowan's characteristic volume
- pc: Critical Pressure
- tb: Normal Boiling Point Temperature
- tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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