

dl-Aspartic acid

Other names:	Aspartic acid, dl- DL-Asparagic acid Aspartic acid acid D,L-aspart
Inchi:	InChI=1S/C4H7NO4/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H,6,7)(H,8,9)
InchiKey:	CKLJMWZTZZHCS-UHFFFAOYSA-N
Formula:	C4H7NO4
SMILES:	NC(CC(=O)O)C(=O)O
Mol. weight [g/mol]:	133.10
CAS:	617-45-8

Physical Properties

Property code	Value	Unit	Source
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/mol×K	811.50	Joback Method
cpg	261.69	J/mol×K	842.78	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C617458&Units=SI

Legend

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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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