

L-Aspartic acid, N-glycyl-

Other names:	N-glycyl-L-aspartic acid
Inchi:	InChI=1S/C6H10N2O5/c7-2-4(9)8-3(6(12)13)1-5(10)11/h3H,1-2,7H2,(H,8,9)(H,10,11)(H,
InchiKey:	SCCPDJAQCXWPTF-GSVOUGTGSA-N
Formula:	C6H10N2O5
SMILES:	NCC(=O)NC(CC(=O)O)C(=O)O
Mol. weight [g/mol]:	190.15
CAS:	4685-12-5

Physical Properties

Property code	Value	Unit	Source
gf	-507.36	kJ/mol	Joback Method
hf	-727.39	kJ/mol	Joback Method
hfus	31.04	kJ/mol	Joback Method
hvap	99.23	kJ/mol	Joback Method
log10ws	0.96		Crippen Method
logp	-2.011		Crippen Method
mcvol	131.810	ml/mol	McGowan Method
pc	5544.32	kPa	Joback Method
tb	804.91	K	Joback Method
tc	1000.89	K	Joback Method
tf	549.73	K	Joback Method
vc	0.485	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.23	J/mol×K	804.91	Joback Method
cpg	382.43	J/mol×K	837.57	Joback Method
cpg	388.16	J/mol×K	870.24	Joback Method
cpg	393.45	J/mol×K	902.90	Joback Method
cpg	398.31	J/mol×K	935.56	Joback Method
cpg	402.74	J/mol×K	968.23	Joback Method
cpg	406.78	J/mol×K	1000.89	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=C4685125&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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