L-Alanine, N-glycyl-

Other names:	Alanine, N-glycyl-, L-
	Gly-ala
	Glycine-«alpha»-alanine
	Glycine-alanine dipeptide
	Glycyl-L-alanine
	Glycylalanine
	N-Glycyl-L-alanine
	N-(Aminoacetyl)alanine, L-
	NSC 83246
	N-glycylalanine
Inchi:	InChI=1S/C5H10N2O3/c1-3(5(9)10)7-4(8)2-6/h3H,2,6H2,1H3,(H,7,8)(H,9,10)/t3-/m1/s1
InchiKey:	VPZXBVLAVMBEQI-GSVOUGTGSA-N
Formula:	C5H10N2O3
SMILES:	CC(NC(=O)CN)C(=O)O
Mol. weight [g/mol]:	146.14
CAS:	3695-73-6

Physical Properties

Property code	Value	Unit	Source
basg	889.10 ± 6.30	kJ/mol	NIST Webbook
basg	888.00 ± 1.20	kJ/mol	NIST Webbook
gf	-250.04	kJ/mol	Joback Method
hf	-441.94	kJ/mol	Joback Method
hfus	22.77	kJ/mol	Joback Method
hvap	73.58	kJ/mol	Joback Method
log10ws	0.47		Crippen Method
logp	-1.466		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
tb	635.98	K	Joback Method
tc	832.14	K	Joback Method
tf	427.71	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.69	J/mol×K	635.98	Joback Method
cpg	291.53	J/mol×K	668.67	Joback Method
cpg	298.92	J/mol×K	701.37	Joback Method
cpg	305.86	J/mol×K	734.06	Joback Method
cpg	312.36	J/mol×K	766.75	Joback Method
cpg	318.45	J/mol×K	799.44	Joback Method
cpg	324.14	J/mol×K	832.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3695736&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

basg:	Gas basicity
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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