gly-gly-ala

Inchi: InChI=1S/C7H13N3O4/c1-4(7(13)14)10-6(12)3-9-5(11)2-8/h4H,2-3,8H2,1H3,(H,9,11)(H,
InchiKey: CCQOOWAONKGYKQ-UHFFFAOYSA-N
Formula: C7H13N3O4
SMILES: CC(NC(=O)CNC(=O)CN)C(=O)O
Mol. weight [g/mol]: 203.20
CAS: 19729-30-7

Physical Properties

Property code	Value	Unit	Source
basg	914.80	kJ/mol	NIST Webbook
gf	-272.73	kJ/mol	Joback Method
hf	-542.33	kJ/mol	Joback Method
hfus	34.64	kJ/mol	Joback Method
hvap	91.22	kJ/mol	Joback Method
log10ws	0.67		Crippen Method
logp	-2.349		Crippen Method
mcvol	150.010	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	785.78	K	Joback Method
tc	986.65	K	Joback Method
tf	552.84	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.08	J/mol×K	785.78	Joback Method
cpg	442.22	J/mol×K	819.26	Joback Method
cpg	449.77	J/mol×K	852.74	Joback Method
cpg	456.75	J/mol×K	886.21	Joback Method
cpg	463.18	J/mol×K	919.69	Joback Method
cpg	469.08	J/mol×K	953.17	Joback Method
cpg	474.47	J/mol×K	986.65	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19729307&Units=SI

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