hexa-L-alanine

Inchi: InChI=1S/C18H32N6O7/c1-7(19)13(25)20-8(2)14(26)21-9(3)15(27)22-10(4)16(28)23-11(
InchiKey: ZLHDFPIXRRJBKM-PAUJSFGCSA-N
Formula: C18H32N6O7
SMILES: CC(N)C(=O)NC(C)C(=O)NC(C)C(=O)NC(C)C(=O)NC(C)C(=O)NC(C)C(=O)O
Mol. weight [g/mol]: 444.48
CAS: 111652-29-0

Physical Properties

Property code	Value	Unit	Source
basg	981.30	kJ/mol	NIST Webbook
gf	-310.90	kJ/mol	Joback Method
hf	-973.10	kJ/mol	Joback Method
hfus	65.61	kJ/mol	Joback Method
hvap	153.31	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	-3.058		Crippen Method
mcvol	339.650	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
tb	1347.38	K	Joback Method
tc	1713.37	K	Joback Method
tf	909.58	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1194.60	J/mol×K	1347.38	Joback Method
cpg	1198.05	J/mol×K	1408.38	Joback Method
cpg	1199.61	J/mol×K	1469.38	Joback Method
cpg	1199.58	J/mol×K	1530.38	Joback Method
cpg	1198.26	J/mol×K	1591.37	Joback Method
cpg	1195.95	J/mol×K	1652.37	Joback Method
cpg	1192.94	J/mol×K	1713.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111652290&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