

penta-L-alanine

Inchi:	InChI=1S/C15H27N5O6/c1-6(16)11(21)17-7(2)12(22)18-8(3)13(23)19-9(4)14(24)20-10(5)
InchiKey:	XXAUOPDVAKGRPR-WYCDGMCDSA-N
Formula:	C15H27N5O6
SMILES:	CC(N)C(=O)NC(C)C(=O)NC(C)C(=O)NC(C)C(=O)NC(C)C(=O)O
Mol. weight [g/mol]:	373.40
CAS:	10183-34-3

Physical Properties

Property code	Value	Unit	Source
basg	962.00	kJ/mol	NIST Webbook
gf	-294.19	kJ/mol	Joback Method
hf	-846.79	kJ/mol	Joback Method
hfus	54.67	kJ/mol	Joback Method
hvap	133.84	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	-2.563		Crippen Method
mcvol	285.830	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
tb	1175.14	K	Joback Method
tc	1449.06	K	Joback Method
tf	788.18	K	Joback Method
vc	1.063	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.42	J/molxK	1175.14	Joback Method
cpg	990.25	J/molxK	1220.79	Joback Method
cpg	995.77	J/molxK	1266.45	Joback Method
cpg	1000.07	J/molxK	1312.10	Joback Method
cpg	1003.27	J/molxK	1357.75	Joback Method
cpg	1005.47	J/molxK	1403.40	Joback Method
cpg	1006.78	J/molxK	1449.06	Joback Method

Sources

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=C10183343&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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