

cycloheximide

Inchi:	InChI=1S/C15H23NO4/c1-8-3-9(2)15(20)11(4-8)12(17)5-10-6-13(18)16-14(19)7-10/h8-1
InchiKey:	YPHMISFOHDHNIV-UHFFFAOYSA-N
Formula:	C15H23NO4
SMILES:	CC1CC(C)C(=O)C(C(O)CC2CC(=O)NC(=O)C2)C1
Mol. weight [g/mol]:	281.35

Physical Properties

Property code	Value	Unit	Source
gf	-310.42	kJ/mol	Joback Method
hf	-817.77	kJ/mol	Joback Method
hfus	29.10	kJ/mol	Joback Method
hvap	85.01	kJ/mol	Joback Method
log10ws	-1.13		Estimated Solubility Method
log10ws	-1.13		Aqueous Solubility Prediction Method
logp	1.042		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
tb	916.11	K	Joback Method
tc	1156.89	K	Joback Method
tf	620.60	K	Joback Method
vc	0.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.02	J/molxK	916.11	Joback Method
cpg	810.95	J/molxK	956.24	Joback Method
cpg	823.47	J/molxK	996.37	Joback Method
cpg	833.48	J/molxK	1036.50	Joback Method
cpg	840.88	J/molxK	1076.63	Joback Method
cpg	845.60	J/molxK	1116.76	Joback Method
cpg	847.54	J/molxK	1156.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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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