Spiro[cyclooctane-1,5'(6'H)-pyrimidine]-2',4',6'(1'H

Other names: cyclooctyl-5-spirobarbituric acid
Inchi: InChI=1S/C11H16N2O3/c14-8-11(9(15)13-10(16)12-8)6-4-2-1-3-5-7-11/h1-7H2,(H2,12,1
InchiKey: RQNKKIXVVHCBKY-UHFFFAOYSA-N
Formula: C11H16N2O3
SMILES: O=C1NC(=O)C2(CCCCCCC2)C(=O)N1
Mol. weight [g/mol]: 224.26

Physical Properties

Property code	Value	Unit	Source
gf	-111.59	kJ/mol	Joback Method
hf	-469.79	kJ/mol	Joback Method
hfus	16.16	kJ/mol	Joback Method
hvap	66.52	kJ/mol	Joback Method
log10ws	-2.98		Estimated Solubility Method
log10ws	-2.98		Aqueous Solubility Prediction Method
log10ws	-3.17		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	1.083		Crippen Method
mcvol	168.800	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
tb	799.92	K	Joback Method
tc	1097.98	K	Joback Method
tf	667.83	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.37	J/mol×K	799.92	Joback Method
cpg	564.79	J/mol×K	849.60	Joback Method
cpg	584.49	J/mol×K	899.27	Joback Method
cpg	602.49	J/mol×K	948.95	Joback Method

cpg	618.83	J/mol×K	998.63	Joback Method
cpg	633.52	J/mol×K	1048.30	Joback Method
cpg	646.59	J/mol×K	1097.98	Joback Method

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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