7,9-diazaspiro[4.5]decane-6,8,10-trione

Other names: cyclopentyl-5-spirobarbituric acid
Inchi: InChI=1S/C8H10N2O3/c11-5-8(3-1-2-4-8)6(12)10-7(13)9-5/h1-4H2,(H2,9,10,11,12,13)
InchiKey: HYPRUQJUBWRVEM-UHFFFAOYSA-N
Formula: C8H10N2O3
SMILES: O=C1NC(=O)C2(CCCC2)C(=O)N1
Mol. weight [g/mol]: 182.18

Physical Properties

Property code	Value	Unit	Source
gf	-100.55	kJ/mol	Joback Method
hf	-389.39	kJ/mol	Joback Method
hfus	14.69	kJ/mol	Joback Method
hvap	59.33	kJ/mol	Joback Method
log10ws	-2.35		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-2.35		Estimated Solubility Method
log10ws	-2.35		Aqueous Solubility Prediction Method
logp	-0.087		Crippen Method
mcvol	126.530	ml/mol	McGowan Method
pc	5153.45	kPa	Joback Method
tb	718.47	K	Joback Method
tc	1012.20	K	Joback Method
tf	644.58	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.92	J/mol×K	718.47	Joback Method
cpg	388.44	J/mol×K	767.42	Joback Method
cpg	404.97	J/mol×K	816.38	Joback Method
cpg	420.56	J/mol×K	865.33	Joback Method

cpg	435.29	J/mol×K	914.29	Joback Method
cpg	449.20	J/mol×K	963.24	Joback Method
cpg	462.36	J/mol×K	1012.20	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