5,7-Diazaspiro[2.5]octane-4,6,8-trione

Other names: cyclopropyl-5-spirobarbituric acid
Inchi: InChI=1S/C6H6N2O3/c9-3-6(1-2-6)4(10)8-5(11)7-3/h1-2H2,(H2,7,8,9,10,11)
InchiKey: PQVZDTWRGIHYCU-UHFFFAOYSA-N
Formula: C6H6N2O3
SMILES: O=C1NC(=O)C2(CC2)C(=O)N1
Mol. weight [g/mol]: 154.13

Physical Properties

Property code	Value	Unit	Source
gf	-93.19	kJ/mol	Joback Method
hf	-335.79	kJ/mol	Joback Method
hfus	13.71	kJ/mol	Joback Method
hvap	54.53	kJ/mol	Joback Method
log10ws	-1.89		Estimated Solubility Method
log10ws	-1.89		Aqueous Solubility Prediction Method
log10ws	-1.89		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-0.867		Crippen Method
mcvol	98.350	ml/mol	McGowan Method
pc	6389.77	kPa	Joback Method
tb	664.17	K	Joback Method
tc	953.82	K	Joback Method
tf	629.08	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.48	J/mol×K	664.17	Joback Method
cpg	280.21	J/mol×K	712.44	Joback Method
cpg	293.33	J/mol×K	760.72	Joback Method
cpg	305.95	J/mol×K	808.99	Joback Method

cpg	318.13	J/mol×K	857.27	Joback Method
cpg	329.96	J/mol×K	905.54	Joback Method
cpg	341.53	J/mol×K	953.82	Joback Method

Sources

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
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/

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