2,4-diazaspiro[5.5]undecane-1,3,5-trione

Other names: cyclohexyl-5-spirobarbituric acid
Inchi: InChI=1S/C9H12N2O3/c12-6-9(4-2-1-3-5-9)7(13)11-8(14)10-6/h1-5H2,(H2,10,11,12,13,1
InchiKey: NBLIVIWUPTWDMD-UHFFFAOYSA-N
Formula: C9H12N2O3
SMILES: O=C1NC(=O)C2(CCCCC2)C(=O)N1
Mol. weight [g/mol]: 196.21

Physical Properties

Property code	Value	Unit	Source
gf	-104.23	kJ/mol	Joback Method
hf	-416.19	kJ/mol	Joback Method
hfus	15.18	kJ/mol	Joback Method
hvap	61.73	kJ/mol	Joback Method
log10ws	-3.06		Estimated Solubility Method
log10ws	-3.06		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-3.06		Aqueous Solubility Prediction Method
logp	0.303		Crippen Method
mcvol	140.620	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
tb	745.62	K	Joback Method
tc	1041.00	K	Joback Method
tf	652.33	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.50	J/mol×K	745.62	Joback Method
cpg	445.57	J/mol×K	794.85	Joback Method
cpg	463.43	J/mol×K	844.08	Joback Method
cpg	480.12	J/mol×K	893.31	Joback Method

cpg	495.70	J/mol×K	942.54	Joback Method
cpg	510.20	J/mol×K	991.77	Joback Method
cpg	523.67	J/mol×K	1041.00	Joback Method

Sources

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/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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