Cycloheptyl-5-spirobarbituric acid

Inchi: InChI=1S/C10H14N2O3/c13-7-10(5-3-1-2-4-6-10)8(14)12-9(15)11-7/h1-6H2,(H2,11,12,1
InchiKey: RSWPVXFVQHCCCI-UHFFFAOYSA-N
Formula: C10H14N2O3
SMILES: O=C1NC(=O)C2(CCCCCC2)C(=O)N1
Mol. weight [g/mol]: 210.23

Physical Properties

Property code	Value	Unit	Source
gf	-107.91	kJ/mol	Joback Method
hf	-442.99	kJ/mol	Joback Method
hfus	15.67	kJ/mol	Joback Method
hvap	64.13	kJ/mol	Joback Method
log10ws	-3.17		Aqueous Solubility Prediction Method
log10ws	-3.17		Estimated Solubility Method
logp	0.693		Crippen Method
mcvol	154.710	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
tb	772.77	K	Joback Method
tc	1069.58	K	Joback Method
tf	660.08	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.05	J/mol×K	772.77	Joback Method
cpg	504.43	J/mol×K	822.24	Joback Method
cpg	523.35	J/mol×K	871.71	Joback Method
cpg	540.85	J/mol×K	921.18	Joback Method
cpg	556.97	J/mol×K	970.65	Joback Method
cpg	571.73	J/mol×K	1020.12	Joback Method
cpg	585.18	J/mol×K	1069.58	Joback Method

Sources

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
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

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