5,5-dimethylbarbituric acid

Inchi: InChI=1S/C6H8N2O3/c1-6(2)3(9)7-5(11)8-4(6)10/h1-2H3,(H2,7,8,9,10,11)
InchiKey: LAOZSCRCYVBSJA-UHFFFAOYSA-N
Formula: C6H8N2O3
SMILES: CC1(C)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 156.14

Physical Properties

Property code	Value	Unit	Source
gf	-173.75	kJ/mol	Joback Method
hf	-435.09	kJ/mol	Joback Method
hfus	14.54	kJ/mol	Joback Method
hvap	54.48	kJ/mol	Joback Method
log10ws	-1.74		Estimated Solubility Method
log10ws	-1.74		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-1.74		Aqueous Solubility Prediction Method
logp	-0.621		Crippen Method
mcvol	109.210	ml/mol	McGowan Method
pc	5183.17	kPa	Joback Method
tb	657.03	K	Joback Method
tc	936.00	K	Joback Method
tf	603.38	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.98	J/mol×K	657.03	Joback Method
cpg	301.81	J/mol×K	703.53	Joback Method
cpg	316.03	J/mol×K	750.02	Joback Method
cpg	329.63	J/mol×K	796.52	Joback Method
cpg	342.56	J/mol×K	843.01	Joback Method

cpg	354.82	J/mol×K	889.51	Joback Method
cpg	366.38	J/mol×K	936.00	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=T999917689&Units=SI&Mask=3FFF
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

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