5,5-Diisopropylbarbituric acid

Other names: 5,5-diisopropylbarbital
Inchi: InChI=1S/C10H16N2O3/c1-5(2)10(6(3)4)7(13)11-9(15)12-8(10)14/h5-6H,1-4H3,(H2,11,1
InchiKey: NSQYIEOSFPLTJA-UHFFFAOYSA-N
Formula: C10H16N2O3
SMILES: CC(C)C1(C(C)C)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 212.25

Physical Properties

Property code	Value	Unit	Source
gf	-144.95	kJ/mol	Joback Method
hf	-528.21	kJ/mol	Joback Method
hfus	17.86	kJ/mol	Joback Method
hvap	62.61	kJ/mol	Joback Method
log10ws	-2.77		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-2.77		Estimated Solubility Method
log10ws	-2.77		Aqueous Solubility Prediction Method
logp	0.651		Crippen Method
mcvol	165.570	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
tb	747.67	K	Joback Method
tc	1010.94	K	Joback Method
tf	618.46	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.56	J/mol×K	747.67	Joback Method
cpg	514.13	J/mol×K	791.55	Joback Method
cpg	531.68	J/mol×K	835.43	Joback Method
cpg	548.23	J/mol×K	879.31	Joback Method

cpg	563.76	J/mol×K	923.18	Joback Method
cpg	578.30	J/mol×K	967.06	Joback Method
cpg	591.83	J/mol×K	1010.94	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
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