5-allyl-5-methyl-barbituric acid

Other names: 5-allyl-5-methylbarbital
Inchi: InChI=1S/C8H10N2O3/c1-3-4-8(2)5(11)9-7(13)10-6(8)12/h3H,1,4H2,2H3,(H2,9,10,11,12
InchiKey: WMSQREUDUHHDDC-UHFFFAOYSA-N
Formula: C8H10N2O3
SMILES: C=CCC1(C)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 182.18

Physical Properties

Property code	Value	Unit	Source
gf	-69.07	kJ/mol	Joback Method
hf	-350.94	kJ/mol	Joback Method
hfus	18.44	kJ/mol	Joback Method
hvap	58.27	kJ/mol	Joback Method
log10ws	-1.16		Estimated Solubility Method
log10ws	-1.16		Aqueous Solubility Prediction Method
log10ws	-1.16		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-0.065		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
tb	699.47	K	Joback Method
tc	970.45	K	Joback Method
tf	624.16	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.29	J/mol×K	699.47	Joback Method
cpg	380.17	J/mol×K	744.63	Joback Method
cpg	395.29	J/mol×K	789.80	Joback Method
cpg	409.65	J/mol×K	834.96	Joback Method

cpg	423.27	J/mol×K	880.12	Joback Method
cpg	436.14	J/mol×K	925.29	Joback Method
cpg	448.25	J/mol×K	970.45	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