5-ethyl-5-methyl-1,3-diazinane-2,4,6-trione

Other names: 5-methyl-5-ethylbarbituric acid
Inchi: InChI=1S/C7H10N2O3/c1-3-7(2)4(10)8-6(12)9-5(7)11/h3H2,1-2H3,(H2,8,9,10,11,12)
InchiKey: RCFRTWDBBMGLGK-UHFFFAOYSA-N
Formula: C7H10N2O3
SMILES: CCC1(C)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 170.17

Physical Properties

Property code	Value	Unit	Source
gf	-165.33	kJ/mol	Joback Method
hf	-455.73	kJ/mol	Joback Method
hfus	17.13	kJ/mol	Joback Method
hvap	56.71	kJ/mol	Joback Method
log10ws	-1.16		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-1.23		Estimated Solubility Method
log10ws	-1.23		Aqueous Solubility Prediction Method
logp	-0.231		Crippen Method
mcvol	123.300	ml/mol	McGowan Method
pc	4534.68	kPa	Joback Method
tb	679.91	K	Joback Method
tc	951.71	K	Joback Method
tf	614.65	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.63	J/mol×K	679.91	Joback Method
cpg	352.44	J/mol×K	725.21	Joback Method
cpg	367.54	J/mol×K	770.51	Joback Method
cpg	381.92	J/mol×K	815.81	Joback Method

cpg	395.57	J/mol×K	861.11	Joback Method
cpg	408.48	J/mol×K	906.41	Joback Method
cpg	420.62	J/mol×K	951.71	Joback Method

Sources

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
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

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