1,3-Dimethylbarbituric acid

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 1,3-dimethyl- Barbituric acid, 1,3-dimethyl- N,N'-Dimethylbarbituric acid
Inchi:	InChI=1S/C6H8N2O3/c1-7-4(9)3-5(10)8(2)6(7)11/h3H2,1-2H3
InchiKey:	VVSASNKOFCZVES-UHFFFAOYSA-N
Formula:	C6H8N2O3
SMILES:	CN1C(=O)CC(=O)N(C)C1=O
Mol. weight [g/mol]:	156.14
CAS:	769-42-6

Physical Properties

Property code	Value	Unit	Source
hfus	17.70	kJ/mol	Thermophysical Study of Several Barbituric Acid Derivatives by Differential Scanning Calorimetry (DSC)
log10ws	0.33		Crippen Method
logp	-0.573		Crippen Method
mcvol	109.210	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C769426&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermophysical Study of Several Barbituric Acid Derivatives by Differential Scanning Calorimetry (DSC) :	https://www.doi.org/10.1021/je1008944

Legend

hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume