1,5-Dimethylbarbituric acid

Inchi: InChI=1S/C6H8N2O3/c1-3-4(9)7-6(11)8(2)5(3)10/h3H,1-2H3,(H,7,9,11)
InchiKey: DABBHRQKJNIVFT-UHFFFAOYSA-N
Formula: C6H8N2O3
SMILES: CC1C(=O)NC(=O)N(C)C1=O
Mol. weight [g/mol]: 156.14
CAS: 7391-67-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.05		Crippen Method
logp	-0.669		Crippen Method
mcvol	109.210	ml/mol	McGowan Method
tf	446.00 ± 4.00	K	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7391675&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.