Thiobarbital Me

Inchi: InChI=1S/C10H16N2O2S/c1-5-10(6-2)7(13)11(3)9(15)12(4)8(10)14/h5-6H2,1-4H3
InchiKey: FVECWDUCSHUMJX-UHFFFAOYSA-N
Formula: C10H16N2O2S
SMILES: CCC1(CC)C(=O)N(C)C(=S)N(C)C1=O
Mol. weight [g/mol]: 228.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.70		Crippen Method
logp	1.008		Crippen Method
mcvol	176.050	ml/mol	McGowan Method
rinpol	1679.00		NIST Webbook
rinpol	1679.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R40582&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
rinpol: Non-polar retention indices

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