2,4,6(1H,3H,5H)-Pyrimidinetrione, 1,3-dimethyl-5-(1-methylbutyl)-5-(2-propenyl)-

Other names: Barbituric acid, 5-allyl-1,3-dimethyl-5-(1-methylbutyl)-
N,N-Dimethylquinalbarbitone
1,3-Dimethylsecobarbital
5-Allyl-1,3-dimethyl-5-(1-methylbutyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
Secobarbital, 1,3-dimethyl
Secobarbital, (bis-Me)
Secobarbital permethylated
Secobarbital Me

Inchi: InChI=1S/C14H22N2O3/c1-6-8-10(3)14(9-7-2)11(17)15(4)13(19)16(5)12(14)18/h7,10H,2

InchiKey: KKPCLTFASPTTIQ-UHFFFAOYSA-N

Formula: C14H22N2O3

SMILES: C=CCC1(C(C)CCC)C(=O)N(C)C(=O)N(C)C1=O

Mol. weight [g/mol]: 266.34

CAS: 28239-49-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	2.035		Crippen Method
mcvol	217.630	ml/mol	McGowan Method
rinpol	1680.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1670.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28239498&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