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

Other names: Barbituric acid, 5-ethyl-5-isopentyl-1,3-dimethyl-
Dimethylamobarbital
N,N'-Dimethylamobarbital
1,3-Dimethyl derivative of amobarbital
Amylobarbitone-permethylated
5-Ethyl-5-isopentyl-1,3-dimethyl-2,4,6(1H,3H,5H)-pyrimidinetrione
Amobarbital, 1,3-dimethyl
Amobarbital, (bis-Me)
Amobarbital permethylated
Amobarbital Me

Inchi: InChI=1S/C13H22N2O3/c1-6-13(8-7-9(2)3)10(16)14(4)12(18)15(5)11(13)17/h9H,6-8H2,1

InchiKey: SETFOBQXPZJCGE-UHFFFAOYSA-N

Formula: C13H22N2O3

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

Mol. weight [g/mol]: 254.33

CAS: 28239-46-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	1.869		Crippen Method
mcvol	207.840	ml/mol	McGowan Method
rinpol	1614.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1590.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28239465&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