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

Other names: Barbituric acid, 5-ethyl-1,3-dimethyl-5-(1-methylbutyl)-
Dimethylpentobarbital
N,N'-Dimethylpentobarbital
Barbituric acid, 1,3-dimethyl-5-ethyl-5-(1-methylbutyl)-
1,3-Dimethyl-5-ethyl-5-(1-methylbutyl)barbituric acid
1,3-Dimethylpentobarbital
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-1,3-dimethyl-5-(1-methylbuthyl)-
Pentobarbitone-permethylated
1,3-Dimethyl derivative of pentobarbital
5-Ethyl-1,3-dimethyl-5-(1-methylbutyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
Pentobarbital, 1,3-dimethyl
Pentobarbital permethylated

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

InchiKey: VZZFPHAKJNPXQY-UHFFFAOYSA-N

Formula: C13H22N2O3

SMILES: CCCC(C)C1(CC)C(=O)N(C)C(=O)N(C)C1=O

Mol. weight [g/mol]: 254.33

CAS: 28239-47-6

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	1618.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1632.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28239476&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices