Dimethylphenobarbital

Other names: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-1,3-dimethyl-5-phenyl-
Barbituric acid, 5-ethyl-1,3-dimethyl-5-phenyl-
N,N'-Dimethylphenobarbital
1,3-Dimethylphenobarbital
1,3-Dimethylphenobarbitone
Barbituric acid, 1,3-dimethyl-5-ethyl-5-phenyl-
1,3-Dimethyl-5-ethyl-5-phenylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 1,3-dimethyl-5-ethyl-5-phenyl-
5-Ethyl-1,3-dimethyl-5-phenylbarbituric acid
1,3-Dimethyl derivative of Phenobarbitol
Phenobarbitone-permethylated
Methylphenobarbitone-permethylated
N,N-Dimethyl-5-ethyl-5-phenylbarbituric acid
Phenobarbital di-methyl derivative
Mephobarbital Me
Mephobarbital permethylated
Phenobarbital, 1,3-dimethyl
Phenobarbital, permethyl
Phenobarbital permethylated
Methylphenobarbital, permethylated
Phenobarbital Me

Inchi: InChI=1S/C14H16N2O3/c1-4-14(10-8-6-5-7-9-10)11(17)15(2)13(19)16(3)12(14)18/h5-9H

InchiKey: RPJARFKGODFVHL-UHFFFAOYSA-N

Formula: C14H16N2O3

SMILES: CCC1(c2ccccc2)C(=O)N(C)C(=O)N(C)C1=O

Mol. weight [g/mol]: 260.29

CAS: 730-66-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.80		Crippen Method
logp	1.385		Crippen Method
mcvol	198.170	ml/mol	McGowan Method
rinpol	1881.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1880.00		NIST Webbook

rinpol	1880.00	NIST Webbook
rinpol	1881.00	NIST Webbook
rinpol	1831.00	NIST Webbook
rinpol	1826.00	NIST Webbook
rinpol	1825.00	NIST Webbook
rinpol	1881.00	NIST Webbook
rinpol	1832.00	NIST Webbook
rinpol	1832.00	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C730665&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices