Mephobarbital

Other names:

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-1-methyl-5-phenyl-
Barbituric acid, 5-ethyl-1-methyl-5-phenyl-
Enfenemal
Enphenemal
Isonal
Isonal (Roussel)
Mebaral
Mephobarbitone
Mephytal
Methyl phenobarbitone
Methyl-calminal
Methylphenobarbital
Metylfenemal
Metyna
Morbusan
N-Methyl-5-phenyl-5-ethylbarbituric acid
N-Methylethylphenylbarbituric acid
N-Methylphenobarbital
Phemetone
Phemiton
Phemitone
Prominal
1-Methylphenobarbital
N-Ethylmethylphenylbarbituric acid
5-Ethyl-N-methyl-5-phenylbarbituric acid
5-Ethyl-1-methyl-5-phenylbarbituric acid
5-Ethyl-5-phenyl-N-methyl-bartituric acid
Meberal
Menta-bal
1-Methyl-5-ethyl-5-phenylbarbituric acid
N-Methylphenolbarbitol
Methylphenylbarbituric acid
N-Methyl-5-phenyl-5-ethylbarbital
1-Methyl-5-phenyl-5-ethylbarbituric acid
5-Phenyl-5-ethyl-3-methylbarbituric acid
5-Ethyl-1-methyl-5-phenyl-2,4,6(1H,3H,5H)-pyrimidinetrione
1-Methyl-5-ethyl-5-phenyl-pyrimidine-2,4,6-trione
Hexahydropyrimidine-2,4,6-trione,1-methyl-5-ethyl-5-phenyl-
Phenobarbital, mono-methyl
(.+/-.)-Mephobarbital

Inchi: InChI=1S/C13H14N2O3/c1-3-13(9-7-5-4-6-8-9)10(16)14-12(18)15(2)11(13)17/h4-8H,3H2

InchiKey: ALARQZQTBTVLJV-UHFFFAOYSA-N

Formula: C13H14N2O3

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

Mol. weight [g/mol]: 246.26

CAS: 115-38-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	1.043		Crippen Method
mcvol	184.080	ml/mol	McGowan Method
rinpol	1883.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1898.00		NIST Webbook
rinpol	1888.00		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1874.00		NIST Webbook
rinpol	1876.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1891.00		NIST Webbook
rinpol	1874.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1883.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1891.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1869.00		NIST Webbook

Sources

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=C115388&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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