2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-1-methyl-5-phenyl-

Other names:

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

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]: 246.27

Physical Properties

Property code	Value	Unit	Source
ie	8.97	eV	Cheméo Relay (1.0)
log10ws	-2.57		Cheméo Relay (1.0)
logp	1.043		Crippen Method
mcvol	184.080	ml/mol	McGowan Method
tf	472.95	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C115388&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.