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

Other names: 1-Methyl-5,5-diethyl barbituric acid
1-Methylbarbital
5,5-Diethyl-1-methyl-2,4,6(1H,3H,5H)-pyrimidinetrione
5,5-Diethyl-1-methyl-2,4,6-trioxo-hexahydropyrimidine
5,5-Diethyl-1-methylbarbituric acid
AN 23
Barbituric acid, 5,5-diethyl-1-methyl-
Endiemal
Endiemalum
Gemonal
Gemonil
Gemonit
Metabarbital
Methabarbitone
Metharbitone
Metharbutal
Methylbarbital
N-Methylbarbital
NSC 27156
Sch 412
metharbital

Inchi: InChI=1S/C9H14N2O3/c1-4-9(5-2)6(12)10-8(14)11(3)7(9)13/h4-5H2,1-3H3,(H,10,12,14)

InchiKey: FWJKNZONDWOGMI-UHFFFAOYSA-N

Formula: C9H14N2O3

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

Mol. weight [g/mol]: 198.22

Physical Properties

Property code	Value	Unit	Source
ie	9.38	eV	Cheméo Relay (1.0)
log10ws	-2.10		Aqueous Solubility Prediction Method
log10ws	-2.23		Estimated Solubility Method
logp	0.501		Crippen Method
mcvol	151.480	ml/mol	McGowan Method
rinpol	1421.00		NIST Webbook

rinpol	1417.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1472.20		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1417.00		NIST Webbook
tf	423.65	K	Aqueous Solubility Prediction Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50113&Units=SI

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

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

Legend

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