Metharbital

Other names:	1-Methyl-5,5-diethyl barbituric acid
	1-Methylbarbital
	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-diethyl-1-methyl-
	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
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
CAS:	50-11-3

Physical Properties

Property code	Value	Unit	Source
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	1417.00		NIST Webbook

rinpol	1417.00		NIST Webbook
rinpol	1421.00		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
tf	423.65	K	Aqueous Solubility Prediction Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50113&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
tf: Normal melting (fusion) point