Hexobarbital

Other names:	1,5-Dimethyl-5-(1-cyclohexenyl)barbituric acid
	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-cyclohexen-1-yl)-1,5-dimethyl-
	5-(1-Cyclohexen-1-yl)-1,5-dimethyl-2,4,6(1H,3H,5H)-pyrimidinetrione
	5-(1-Cyclohexen-1-yl)-1,5-dimethylbarbituric acid
	5-(1-Cyclohexenyl-1)-1-methyl-5-methylbarbituric acid
	5-(Cyclohexen-1-yl)-1,5-dimethylbarbituric acid
	5-(Cyclohexen-1-yl)-1,5-dimethylbarbitursaeure
	5-(«delta»-1,2-cyclohexenyl)-5-methyl-N-methyl-barbitursaeure
	5-(Â«deltaÂ»-1,2-cyclohexenyl)-5-methyl-N-methyl-barbitursaeure
	Barbidorm
	Barbituric acid, 5-(1-cyclohexen-1-yl)-1,5-dimethyl-
	Citodon
	Citopan
	Cyclonal
	Cyclopan
	Dorico
	Enhexymal
	Esobarbitale
	Evipal
	Evipan
	Hexabarbital
	Hexanastab oral
	Hexenal
	Hexenal (barbiturate)
	Hexobarbitone
	Methexenyl
	Methylhexabarbital
	Methylhexabital
	N-Methyl-5-cyclohexenyl-5-methylbarbituric acid
	NSC 71929
	Narcosan
	Noctivane
	Sombucaps
	Sombulex
	Somnalert
Inchi:	InChI=1S/C12H16N2O3/c1-12(8-6-4-3-5-7-8)9(15)13-11(17)14(2)10(12)16/h6H,3-5,7H2,
InchiKey:	UYXAWHWODHRRMR-UHFFFAOYSA-N
Formula:	C12H16N2O3
SMILES:	CN1C(=O)NC(=O)C(C)(C2=CCCCC2)C1=O
Mol. weight [g/mol]:	236.27

CAS: 56-29-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.67		Aqueous Solubility Prediction Method
logp	1.201		Crippen Method
mcvol	178.590	ml/mol	McGowan Method
rinpol	1850.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1904.30		NIST Webbook
rinpol	1862.00		NIST Webbook
rinpol	1817.00		NIST Webbook
rinpol	1831.00		NIST Webbook
rinpol	1831.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1853.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1839.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1845.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1857.00		NIST Webbook
rinpol	1851.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1857.00		NIST Webbook

rinpol	1860.00		NIST Webbook
tf	365.48	K	Aqueous Solubility Prediction Method
tf	418.00 ± 4.00	K	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56291&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