

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-cyclohexen-1-yl)-1,3,5-trimethyl-

Other names:	Barbituric acid, 5-(1-cyclohexen-1-yl)-1,3,5-trimethyl- 3-Methyl derivative of Hexobarbital Hexobarbital Me Hexobarbital permethylated
Inchi:	InChI=1S/C13H18N2O3/c1-13(9-7-5-4-6-8-9)10(16)14(2)12(18)15(3)11(13)17/h7H,4-6,8
InchiKey:	PCTJGZPAPPNSKM-UHFFFAOYSA-N
Formula:	C13H18N2O3
SMILES:	CN1C(=O)N(C)C(=O)C(C)(C2=CCCCC2)C1=O
Mol. weight [g/mol]:	250.29
CAS:	726-79-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	1.543		Crippen Method
mcvol	192.680	ml/mol	McGowan Method
rinpol	1833.00		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1795.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C726794&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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