

3,5-Dimethyl-5-(3-oxocyclohex-1-enyl)-hexahydro

Other names:	3'-Keto hexobarbital 3'-Oxohexobarbital Hexobarbital M (oxo)
Inchi:	InChI=1S/C12H14N2O4/c1-12(7-4-3-5-8(15)6-7)9(16)13-11(18)14(2)10(12)17/h6H,3-5H2
InchiKey:	JLDHHLBFGIBRGN-UHFFFAOYSA-N
Formula:	C12H14N2O4
SMILES:	CN1C(=O)NC(=O)C(C)(C2=CC(=O)CCC2)C1=O
Mol. weight [g/mol]:	250.25
CAS:	427-30-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.59		Crippen Method
logp	0.380		Crippen Method
mcvol	180.160	ml/mol	McGowan Method
rinpola	2055.00		NIST Webbook
rinpola	2055.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C427305&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpola:	Non-polar retention indices

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