

2,4,6(1H,3H,5H)-Pyrimidinetrione, 1,3-dimethyl-5-(2-methylpropyl)-5-(2-propenyl)-

Other names:	1,3-Dimethyl derivative of butalbital N,N'-Dimethylbutalbital Allylbarbital, 1,3-dimethyl Butalbital, permethylated
Inchi:	InChI=1S/C13H20N2O3/c1-6-7-13(8-9(2)3)10(16)14(4)12(18)15(5)11(13)17/h6,9H,1,7-8
InchiKey:	GDEXVBXMOVNKKD-UHFFFAOYSA-N
Formula:	C13H20N2O3
SMILES:	<chem>C=CCC1(CC(C)C)C(=O)N(C)C(=O)N(C)C1=O</chem>
Mol. weight [g/mol]:	252.31
CAS:	55045-04-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Crippen Method
logp	1.645		Crippen Method
mcvol	203.540	ml/mol	McGowan Method
rinpol	1553.00		NIST Webbook
rinpol	1553.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55045040&Units=SI

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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