

Mephobarbital M (OH)

Inchi: InChI=1S/C13H14N2O4/c1-8(16)13(9-6-4-3-5-7-9)10(17)14-12(19)15(2)11(13)18/h3-8,10,12,14,16,18,20
InchiKey: QQTAUICLIXCZDS-UHFFFAOYSA-N
Formula: C13H14N2O4
SMILES: CC(O)C1(c2ccccc2)C(=O)NC(=O)N(C)C1=O
Mol. weight [g/mol]: 262.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.37		Crippen Method
logp	0.013		Crippen Method
mcvol	189.950	ml/mol	McGowan Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R57541&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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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