

Mephenytoin perethylated

Inchi: InChI=1S/C14H18N2O2/c1-4-14(11-9-7-6-8-10-11)12(17)15(3)13(18)16(14)5-2/h6-10H,4
InchiKey: ZDRIBPOKVNVS BV-UHFFFAOYSA-N
Formula: C14H18N2O2
SMILES: CCN1C(=O)N(C)C(=O)C1(CC)c1cccc1
Mol. weight [g/mol]: 246.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	2.206		Crippen Method
mcvol	196.600	ml/mol	McGowan Method
rinpol	2339.00		NIST Webbook
rinpol	2339.00		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=R387947&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

Latest version available from:

<https://www.chemeo.com/cid/61-938-3/Mephenytoin-perethylated.pdf>

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