Mephenytoin, M (HO-methoxy-), AC

Inchi: InChI=1S/C15H18N2O5/c1-5-15(13(19)17(3)14(20)16-15)10-6-7-11(22-9(2)18)12(8-10)2
InchiKey: ZYVSKYZLTNNVBD-UHFFFAOYSA-N
Formula: C15H18N2O5
SMILES: CCC1(c2ccc(OC(C)=O)c(OC)c2)NC(=O)N(C)C1=O
Mol. weight [g/mol]: 306.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	1.407		Crippen Method
mcvol	224.000	ml/mol	McGowan Method
rinpol	2630.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R255637&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