Mephenytoin, M (HO-), AC

Inchi: InChI=1S/C14H16N2O4/c1-4-14(12(18)16(3)13(19)15-14)10-5-7-11(8-6-10)20-9(2)17/h5
InchiKey: OETAOBHKEDMWHX-UHFFFAOYSA-N
Formula: C14H16N2O4
SMILES: CCC1(c2ccc(OC(C)=O)cc2)NC(=O)N(C)C1=O
Mol. weight [g/mol]: 276.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	1.399		Crippen Method
mcvol	204.040	ml/mol	McGowan Method
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R255622&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.