Minalobine D

Inchi: InChI=1S/C13H23NO3/c1-3-13(2,16)12(15)17-9-10-6-8-14-7-4-5-11(10)14/h10-11,16H,3
InchiKey: CRCCVTJWODFWJV-KKPNGEORSA-N
Formula: C13H23NO3
SMILES: CCC(C)(O)C(=O)OCC1CCN2CCCC12
Mol. weight [g/mol]: 241.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.73		Crippen Method
logp	1.175		Crippen Method
mcvol	195.600	ml/mol	McGowan Method
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook

Sources

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=R414292&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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