Minalobine A

Inchi: InChI=1S/C11H19NO3/c1-8(13)11(14)15-7-9-4-6-12-5-2-3-10(9)12/h8-10,13H,2-7H2,1H3
InchiKey: IPJNFZDILNKMFH-VXRWAFEHSA-N
Formula: C11H19NO3
SMILES: CC(O)C(=O)OCC1CCN2CCCC12
Mol. weight [g/mol]: 213.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.89		Crippen Method
logp	0.395		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
rinpol	1540.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R414267&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