

Minalobine B

Inchi: InChI=1S/C13H21NO2/c1-3-10(2)13(15)16-9-11-6-8-14-7-4-5-12(11)14/h3,11-12H,4-9H2
InchiKey: NWPCVTQQFKZNSF-IPANGIIDSA-N
Formula: C13H21NO2
SMILES: CC=C(C)C(=O)OCC1CCN2CCCC12
Mol. weight [g/mol]: 223.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.21		Crippen Method
logp	1.980		Crippen Method
mcvol	185.430	ml/mol	McGowan Method
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R414272&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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

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