Minalobine I

Inchi: InChI=1S/C16H27NO5/c1-4-14(18)22-11(2)16(3,20)15(19)21-10-12-7-9-17-8-5-6-13(12)1
InchiKey: RVTARTUVJMTYMU-LGESCRJUSA-N
Formula: C16H27NO5
SMILES: CCC(=O)OC(C)C(C)(O)C(=O)OCC1CCN2CCCC12
Mol. weight [g/mol]: 313.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Crippen Method
logp	1.107		Crippen Method
mcvol	245.310	ml/mol	McGowan Method
rinpol	2049.00		NIST Webbook
rinpol	2049.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R414341&Units=SI
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

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.