Minalobine O

Inchi: InChI=1S/C18H29NO5/c1-5-12(2)16(20)24-13(3)18(4,22)17(21)23-11-14-8-10-19-9-6-7-1
InchiKey: QWLVLKBPONBFQZ-LABHKYKLSA-N
Formula: C18H29NO5
SMILES: CC=C(C)C(=O)OC(C)C(C)(O)C(=O)OCC1CCN2CCCC12
Mol. weight [g/mol]: 339.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	1.663		Crippen Method
mcvol	269.190	ml/mol	McGowan Method
rinpol	2236.00		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=R414405&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