9-Hydroxyisohexenoylretronecine

Inchi: InChI=1S/C14H21NO3/c1-10(2)3-4-13(17)18-9-11-5-7-15-8-6-12(16)14(11)15/h3,5,12,14
InchiKey: NZTFQXQFIBMKBH-NBFOIZRFSA-N
Formula: C14H21NO3
SMILES: CC(C)=CCC(=O)OCC1=CCN2CCC(O)C12
Mol. weight [g/mol]: 251.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.10		Crippen Method
logp	1.261		Crippen Method
mcvol	201.090	ml/mol	McGowan Method
rinpol	2041.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R405273&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