9-(2-Methylbutylryl)platynecine

Other names: 9-(2-Methylbutyryl) platinecine
Inchi: InChI=1S/C13H23NO3/c1-3-9(2)13(16)17-8-10-4-6-14-7-5-11(15)12(10)14/h9-12,15H,3-
InchiKey: JDZNNMHSMYUKBP-YECOWLKZSA-N
Formula: C13H23NO3
SMILES: CCC(C)C(=O)OCC1CCN2CCC(O)C12
Mol. weight [g/mol]: 241.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	1.031		Crippen Method
mcvol	195.600	ml/mol	McGowan Method
rinpol	1803.00		NIST Webbook
rinpol	1803.00		NIST Webbook
rinpol	1803.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R395245&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from: