

9-Isoseneciolyretronecine

Inchi: InChI=1S/C13H19NO3/c1-9(2)7-12(16)17-8-10-3-5-14-6-4-11(15)13(10)14/h3,11,13,15H
InchiKey: JWKCRKAONRDKRV-AMGKYWFPSA-N
Formula: C13H19NO3
SMILES: C=C(C)CC(=O)OCC1=CCN2CCC(O)C12
Mol. weight [g/mol]: 237.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.68		Crippen Method
logp	0.871		Crippen Method
mcvol	187.000	ml/mol	McGowan Method
rinpole	1754.00		NIST Webbook
rinpole	1754.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R405293&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/54-536-7/9-Isoseneciolyretronecine.pdf>

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