Phenylacetylscopine

Inchi: InChI=1S/C16H19NO3/c1-17-12-8-11(9-13(17)16-15(12)20-16)19-14(18)7-10-5-3-2-4-6-
InchiKey: CXCYCFDGKJSNIJ-OWRMTOLYSA-N
Formula: C16H19NO3
SMILES: CN1C2CC(OC(=O)Cc3ccccc3)CC1C1OC12
Mol. weight [g/mol]: 273.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	1.385		Crippen Method
mcvol	203.250	ml/mol	McGowan Method
rinpol	2044.00		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=R546626&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