

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
rinpola	2044.00		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=R546626&Units=SI

Legend

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

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<https://www.chemeo.com/cid/58-316-7/Phenylacetylscopine.pdf>

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