narwedine

Other names:	6H-Benzofuro[3a,3,2-ef][2]benzazepin-6-one, 4a,5,9,10,11,12-hexahydro-3-methoxy-11-methyl-, (4aR,8aR)-rel-
Inchi:	InChI=1S/C17H19NO3/c1-18-8-7-17-6-5-12(19)9-14(17)21-16-13(20-2)4-3-11(10-18)15(
InchiKey:	QENVUHCAYXAROT-UHFFFAOYSA-N
Formula:	C17H19NO3
SMILES:	COc1ccc2c3c1OC1CC(=O)C=CC31CCN(C)C2
Mol. weight [g/mol]:	285.34
CAS:	1668-86-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	2.058		Crippen Method
mcvol	213.040	ml/mol	McGowan Method
rinpol	2414.00		NIST Webbook

Sources

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=C1668866&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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