

narwedine

Other names: 6H-Benzofuro[3a,3,2-ef][2]benzazepin-6-one,
Inchi: 4a,5,9,10,11,12-hexahydro-3-methoxy-11-methyl-(4aR,8aR)-rel
InchiKey: QENVUHCAIXAROT-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: <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=C1668866&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

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<https://www.chemeo.com/cid/63-519-6/narwedine.pdf>

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