Norpluvine

Other names: (1R,3a1S,11bS)-10-Methoxy-2,3a1,4,5,7,11b-hexahydro-1H-pyrrolo[3,2,1-de]phenanthrid
Inchi: InChI=1S/C16H19NO3/c1-20-14-7-11-10(6-13(14)19)8-17-5-4-9-2-3-12(18)15(11)16(9)1
InchiKey: KYCRETLRESMMIM-UHFFFAOYSA-N
Formula: C16H19NO3
SMILES: COc1cc2c(cc1O)CN1CCC3=CCC(O)C2C31
Mol. weight [g/mol]: 273.33
CAS: 517-99-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	1.763		Crippen Method
mcvol	203.250	ml/mol	McGowan Method
rinpol	2556.00		NIST Webbook
rinpol	2556.00		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=C517997&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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