(S)-1,2,3,4-tetrahydro-1-[(3-hydroxy-4-methoxyphe

Other names: Reticuline
Inchi: InChI=1S/C19H23NO4/c1-20-7-6-13-10-19(24-3)17(22)11-14(13)15(20)8-12-4-5-18(23-2
InchiKey: BHLYRWXGMIUIHG-UHFFFAOYSA-N
Formula: C19H23NO4
SMILES: COc1ccc(CC2c3cc(O)c(OC)cc3CCN2C)cc1O
Mol. weight [g/mol]: 329.39
CAS: 485-19-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.37		Crippen Method
logp	2.887		Crippen Method
mcvol	253.650	ml/mol	McGowan Method
rinpol	2841.90		NIST Webbook
rinpol	2841.90		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=C485198&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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