Lycoramine

Inchi: InChI=1S/C17H23NO3/c1-18-8-7-17-6-5-12(19)9-14(17)21-16-13(20-2)4-3-11(10-18)15(
InchiKey: GJRMHIXYLGOZSE-UHFFFAOYSA-N
Formula: C17H23NO3
SMILES: COc1ccc2c3c1OC1CC(O)CCC31CCN(C)C2
Mol. weight [g/mol]: 289.37
CAS: 21133-52-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.32		Crippen Method
logp	2.074		Crippen Method
mcvol	221.640	ml/mol	McGowan Method
rinpol	2423.30		NIST Webbook
rinpol	2365.00		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=C21133528&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