

(.+/-)-Platydesmine

Inchi: InChI=1S/C15H17NO3/c1-15(2,17)12-8-10-13(18-3)9-6-4-5-7-11(9)16-14(10)19-12/h4-7,
InchiKey: OYGWMFMSZPRSPD-UHFFFAOYSA-N
Formula: C15H17NO3
SMILES: COc1c2c(nc3ccccc13)OC(C(C)(C)O)C2
Mol. weight [g/mol]: 259.30
CAS: 7764-73-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.30		Crippen Method
logp	2.318		Crippen Method
mcvol	195.720	ml/mol	McGowan Method
rinpol	2360.90		NIST Webbook
rinpol	2360.90		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=C7764730&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

Latest version available from:

<https://www.chemeo.com/cid/93-563-4/Platydesmine.pdf>

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