6H-Dibenzo[a,g]quinolizine-2,9-diol, 5,8,13,13a-tetrahydro-3,10-dimethoxy-, (.+/-.)-

Other names: Berbine-2,9-diol, 3,10-dimethoxy-, (.+/-.)-
(.+/-.)-Scoulerine
(RS)-Scoulerine
6H-Dibenzo[a,g]quinolizine-2,9-diol, 5,8,13,13a-tetrahydro-3,10-dimethoxy-, (±)-
(±)-Scoulerine
Berbine-2,9-diol, 3,10-dimethoxy-, (±)-
dl-Scoulerine

Inchi: InChI=1S/C19H21NO4/c1-23-17-4-3-11-7-15-13-9-16(21)18(24-2)8-12(13)5-6-20(15)10-

InchiKey: KNWVMRVOBAFFMH-UHFFFAOYSA-N

Formula: C19H21NO4

SMILES: COc1cc2c(cc1O)C1Cc3ccc(OC)c(O)c3CN1CC2

Mol. weight [g/mol]: 327.37

CAS: 6451-72-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.73		Crippen Method
logp	2.770		Crippen Method
mcvol	242.790	ml/mol	McGowan Method
rinpol	3190.30		NIST Webbook
rinpol	3190.30		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6451725&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices