

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/ci9903071
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

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