2H,8H-Benzo[1,2-b:3,4-b']dipyran-2-one, 9,10-dihydro-9-hydroxy-8,8-dimethyl-, (R)-

Other names: 2H,8H-Benzo[1,2-b:3,4-b']dipyran-2-one, 9,10-dihydro-9-hydroxy-8,8-dimethyl-, (R)-(+)-Jatamansinol

Lomatin

Inchi: InChI=1S/C14H14O4/c1-14(2)11(15)7-9-10(18-14)5-3-8-4-6-12(16)17-13(8)9/h3-6,11,15

InchiKey: UJSHBYQGQRPVNO-NSHDSACASA-N

Formula: C14H14O4

SMILES: CC1(C)Oc2ccc3ccc(=O)oc3c2CC1O

Mol. weight [g/mol]: 246.26

CAS: 19380-05-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.57		Crippen Method
logp	1.867		Crippen Method
mcvol	177.520	ml/mol	McGowan Method
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19380053&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