(S)-8-((3,3-Dimethyloxiran-2-yl)methyl)-7-methoxy

Inchi: InChI=1S/C15H16O4/c1-15(2)12(19-15)8-10-11(17-3)6-4-9-5-7-13(16)18-14(9)10/h4-7,1
InchiKey: LSZONYLDFHGRDP-GFCCVEGCSA-N
Formula: C15H16O4
SMILES: COc1ccc2ccc(=O)oc2c1CC1OC1(C)C
Mol. weight [g/mol]: 260.29
CAS: 23971-42-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.82		Crippen Method
logp	2.521		Crippen Method
mcvol	191.610	ml/mol	McGowan Method
rinpol	2257.80		NIST Webbook
rinpol	2257.80		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=C23971428&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