

(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

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