8-(2,3-Dihydroxy-3-methylbutyl)-7-methoxy-2H-ch

Inchi: InChI=1S/C15H18O5/c1-15(2,18)12(16)8-10-11(19-3)6-4-9-5-7-13(17)20-14(9)10/h4-7,1
InchiKey: KGGUASRIGLRPAX-UHFFFAOYSA-N
Formula: C15H18O5
SMILES: COc1ccc2ccc(=O)oc2c1CC(O)C(C)(C)O
Mol. weight [g/mol]: 278.30
CAS: 5673-37-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.36		Crippen Method
logp	1.476		Crippen Method
mcvol	208.340	ml/mol	McGowan Method
rinpol	2445.90		NIST Webbook
rinpol	2432.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5673370&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