7-O-Prenylumbelliferone

Inchi: InChI=1S/C14H14O3/c1-10(2)7-8-16-12-5-3-11-4-6-14(15)17-13(11)9-12/h3-7,9H,8H2,1-
InchiKey: SMHJTSOVVRGDEO-UHFFFAOYSA-N
Formula: C14H14O3
SMILES: CC(C)=CCOc1ccc2ccc(=O)oc2c1
Mol. weight [g/mol]: 230.26
CAS: 10387-50-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.08		Crippen Method
logp	3.138		Crippen Method
mcvol	178.210	ml/mol	McGowan Method
rinpol	2142.40		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2142.40		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10387505&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