5-isopentenyloxy-7-methoxycoumarin

Inchi: InChI=1S/C15H16O4/c1-10(2)6-7-18-13-8-11(17-3)9-14-12(13)4-5-15(16)19-14/h4-6,8-9
InchiKey: HSJZJYCOXHKDBJ-UHFFFAOYSA-N
Formula: C15H16O4
SMILES: COc1cc(OCC=C(C)C)c2ccc(=O)oc2c1
Mol. weight [g/mol]: 260.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.20		Crippen Method
logp	3.147		Crippen Method
mcvol	198.170	ml/mol	McGowan Method
rinpol	2351.00		NIST Webbook

Sources

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=R422298&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices