2H-1-Benzopyran-2-one, 3-(1,1-dimethyl-2-propenyl)-7-hydroxy-6-methoxy-

Other names: Coumarin, 3-(1,1-dimethylallyl)-7-hydroxy-6-methoxy-
3-(1,1-Dimethylallyl)scopoletin
3-(1',1'-Dimethylallyl)scopoletin

Inchi: InChI=1S/C15H16O4/c1-5-15(2,3)10-6-9-7-13(18-4)11(16)8-12(9)19-14(10)17/h5-8,16H,

InchiKey: NEUWPSXOYGGGFO-UHFFFAOYSA-N

Formula: C15H16O4

SMILES: C=CC(C)(C)c1cc2cc(OC)c(O)cc2oc1=O

Mol. weight [g/mol]: 260.29

CAS: 19723-23-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.69		Crippen Method
logp	2.971		Crippen Method
mcvol	198.170	ml/mol	McGowan Method
rinpol	2305.80		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=C19723230&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