Scopoletin, O-acetyl-

Inchi: InChI=1S/C12H10O5/c1-7(13)16-11-6-9-8(5-10(11)15-2)3-4-12(14)17-9/h3-6H,1-2H3
InchiKey: HYCLWDHZALFLJV-UHFFFAOYSA-N
Formula: C12H10O5
SMILES: COc1cc2ccc(=O)oc2cc1OC(C)=O
Mol. weight [g/mol]: 234.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.87		Crippen Method
logp	1.727		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
rinpol	2079.00		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=U374301&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