

Scopoletin, O-acetyl-

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|-----------------------------|---|
| 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 |
| rinsol | 2079.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |
| rinsol: | Non-polar retention indices |

Latest version available from:

<https://www.chemeo.com/cid/22-272-5/Scopoletin-O-acetyl.pdf>

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