

Scopoletin, trimethylsilyl ether

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|-----------------------------|---|
| Other names: | Scopoletin, TMS Scopoletin, tms derivative |
| Inchi: | InChI=1S/C13H16O4Si/c1-15-11-7-9-5-6-13(14)16-10(9)8-12(11)17-18(2,3)4/h5-8H,1-4H |
| InchiKey: | NMJKTIAWKZTMIN-UHFFFAOYSA-N |
| Formula: | C13H16O4Si |
| SMILES: | COc1cc2ccc(=O)oc2cc1O[Si](C)(C)C |
| Mol. weight [g/mol]: | 264.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -5.56 | | Crippen Method |
| logp | 3.015 | | Crippen Method |
| rinpola | 2067.80 | | NIST Webbook |
| rinpola | 2067.80 | | NIST Webbook |

Sources

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|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U333497&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| rinpola: | Non-polar retention indices |

Latest version available from:

<https://www.chemeo.com/cid/118-768-9/Scopoletin-trimethylsilyl-ether.pdf>

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