# Scopoletin, tert-butyldimethylsilyl ether

**Other names:** Scopoletin, tbdms derivative
**Inchi:** InChI=1S/C16H22O4Si/c1-16(2,3)21(5,6)20-14-10-12-11(9-13(14)18-4)7-8-15(17)19-12/
**InchiKey:** DMFWNSMRZNRZKR-UHFFFAOYSA-N
**Formula:** C16H22O4Si
**SMILES:** COc1cc2ccc(=O)oc2cc1O[Si](C)(C)C(C)(C)C
**Mol. weight [g/mol]:** 306.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -6.82 | | Crippen Method |
| logp | 4.186 | | Crippen Method |
| rinpol | 2339.90 | | NIST Webbook |
| rinpol | 2339.90 | | NIST Webbook |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U333496&Units=SI

## Legend

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