

# Scopoletin, tert-butyldimethylsilyl ether

<b>Other names:</b>	Scopoletin, tbdms derivative
<b>Inchi:</b>	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/
<b>InchiKey:</b>	DMFWNSMRZNRZKR-UHFFFAOYSA-N
<b>Formula:</b>	C16H22O4Si
<b>SMILES:</b>	COc1cc2ccc(=O)oc2cc1O[Si](C)(C)C(C)(C)C
<b>Mol. weight [g/mol]:</b>	306.43

## Physical Properties

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

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U333496&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333496&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>rinsol:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/118-767-0/Scopoletin-tert-butyldimethylsilyl-ether.pdf>

Generated by Cheméo on 2024-04-28 12:34:20.472840763 +0000 UTC m=+16596909.393418075.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.