Coniferyl aldehyde, tert-butyldimethylsilyl ether

Other names: Coniferyl aldehyde, tbdms derivative
Inchi: InChI=1S/C16H24O3Si/c1-16(2,3)20(5,6)19-14-10-9-13(8-7-11-17)12-15(14)18-4/h7-12H
InchiKey: RTJRBYNXAVSFEL-BQYQJAHWSA-N
Formula: C16H24O3Si
SMILES: COc1cc(C=CC=O)ccc1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 292.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	4.291		Crippen Method
rinpol	2114.70		NIST Webbook
rinpol	2114.70		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=U352424&Units=SI

Legend

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