

3,5-Dimethoxycinnamic acid, tert-butyldimethylsilyl ester

Other names: 3,5-Dimethoxycinnamic acid, tbdms derivative

Inchi: InChI=1S/C17H26O4Si/c1-17(2,3)22(6,7)21-16(18)9-8-13-10-14(19-4)12-15(11-13)20-5/

InchiKey: OZRSKKBVDIYNJU-CMDGGOBGSA-N

Formula: C17H26O4Si

SMILES: COc1cc(C=CC(=O)O[Si](C)(C)C(C)(C)C)cc(OC)c1

Mol. weight [g/mol]: 322.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	4.265		Crippen Method
rinpol	2279.10		NIST Webbook
rinpol	2279.10		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U352436&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

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/49-744-2/3-5-Dimethoxycinnamic-acid-tert-butyldimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-23 07:18:20.691081594 +0000 UTC m=+16145949.611658906.

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