

3-Methoxycinnamic acid, TBDMS

Inchi: InChI=1S/C16H24O3Si/c1-16(2,3)20(5,6)19-15(17)11-10-13-8-7-9-14(12-13)18-4/h7-12H
InchiKey: PBASFTCYWNLALI-ZHACJKMWSA-N
Formula: C16H24O3Si
SMILES: COc1cccc(C=CC(=O)O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]: 292.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.26		Crippen Method
logp	4.257		Crippen Method
rinpol	2036.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R563567&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/50-538-9/3-Methoxycinnamic-acid-TBDMS.pdf>

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