

Benzenepropanoic acid, 3-hydroxy-4-methoxy, TMS

Inchi: InChI=1S/C16H28O4Si2/c1-18-14-10-8-13(12-15(14)19-21(2,3)4)9-11-16(17)20-22(5,6)7
InchiKey: OZSXDGVSWWHMQS-UHFFFAOYSA-N
Formula: C16H28O4Si2
SMILES: COc1ccc(CCC(=O)O[Si](C)(C)C)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 340.56

Physical Properties

Property code	Value	Unit	Source
log10ws	0.01		Crippen Method
logp	4.220		Crippen Method
rinpol	1872.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R94254&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/15-603-5/Benzenepropanoic-acid-3-hydroxy-4-methoxy-TMS.pdf>

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