

Benzenepropanoic acid, 3-methoxy-4[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names

3-Methoxy-4-(trimethylsilyloxy)trimethylsilyl ester of Benzenepropanoic acid

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

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

Vanillylpropionic acid, di-TMS

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

Vanillylpropionic acid, bis-TMS

3-(4-Hydroxy-3-methoxyphenyl)propionic acid, 2tms derivative

Inchi:

InChI=1S/C16H28O4Si2/c1-18-15-12-13(8-10-14(15)19-21(2,3)4)9-11-16(17)20-22(5,6)7

InchiKey:

GRFQIBLVSXVNI-UHFFFAOYSA-N

Formula:

C16H28O4Si2

SMILES:

COc1cc(CCC(=O)O[Si](C)(C)C)ccc1O[Si](C)(C)C

Mol. weight [g/mol]:

340.56

CAS:

56051-49-1

Physical Properties

Property code	Value	Unit	Source
log10ws	0.01		Crippen Method
logp	4.220		Crippen Method
rinpol	1911.00		NIST Webbook
rinpol	1884.00		NIST Webbook
rinpol	1909.00		NIST Webbook
rinpol	1889.00		NIST Webbook
rinpol	1889.00		NIST Webbook
rinpol	1909.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C56051491&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

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