Trimethylsilyl [3-methoxy-4-(trimethylsilyloxy)phenyl]acetate

Other names: Benzeneacetic acid, 3-methoxy-4-[(trimethylsilyl)oxy]-, trimethylsilyl ester
Homovanillic acid (tms)
Benzeneacetic acid, 4-hydroxy-3-methoxy, bis-TMS
Homovanillic acid, bis-TMS
Homovanillic acid, di-TMS
Phenylacetic acid, 3-methoxy-4-trimethylsilyloxy-, trimethylsilyl ester
Homovalillic acid, bis-TMS
Homovanilic acid, TMS
Benzeneacetic acid, 4-hydroxy-3-methoxy, TMS
Homovanillic acid, 2tms derivative

Inchi: InChI=1S/C15H26O4Si2/c1-17-14-10-12(11-15(16)19-21(5,6)7)8-9-13(14)18-20(2,3)4/h8

InchiKey: PPAQHWGGSXMRBE-UHFFFAOYSA-N

Formula: C15H26O4Si2

SMILES: COc1cc(CC(=O)O[Si](C)(C)C)ccc1O[Si](C)(C)C

Mol. weight [g/mol]: 326.54

CAS: 37148-61-1

Physical Properties

Property code	Value	Unit	Source
logp	3.829		Crippen Method
rinpol	1785.00		NIST Webbook
rinpol	1792.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1783.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1786.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1758.00		NIST Webbook

rinpol	1786.00	NIST Webbook
rinpol	1784.00	NIST Webbook
rinpol	1790.00	NIST Webbook
rinpol	1784.00	NIST Webbook
rinpol	1766.00	NIST Webbook
rinpol	1785.00	NIST Webbook
rinpol	1783.00	NIST Webbook
rinpol	1786.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37148611&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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