

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 Homovanillic 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
log10ws	0.43		Crippen Method
logp	3.829		Crippen Method
rinpol	1758.00		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	1785.00		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1759.00		NIST Webbook

rmpol	1758.00	NIST Webbook
rmpol	1786.00	NIST Webbook
rmpol	1784.00	NIST Webbook
rmpol	1790.00	NIST Webbook
rmpol	1784.00	NIST Webbook
rmpol	1766.00	NIST Webbook
rmpol	1785.00	NIST Webbook
rmpol	1783.00	NIST Webbook
rmpol	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/ci9903071>

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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rmpol: Non-polar retention indices

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