Benzeneacetic acid, 3-methoxy-«alpha»,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names: Vanillylmandelic acid, tris(trimethylsilyl)-
3,4-Dihydroxymandelate O3-methyl, tris(trimethylsilyl) ether
Trimethylsilyl O,O'-bis(trimethylsilyl)vanilmandelate
DL-4-Hydroxy-3-methoxymandelic acid, bis(trimethylsilyl) ether, trimethylsilyl ester
Benzeneacetic acid, «alpha»,4-dihydroxy-3-methoxy, tris-TMS
Mandelic acid, 4-hydroxy-3-methoxy, (3TMS)-
Vanillylmandelic acid, tris-TMS
Vanillylmandelic acid, tri-TMS
Vanilmandelic acid, (3TMS)-
Vanilmandelic acid, triTMS
Mandelic acid, 4-hydroxy-3-methoxy, TMS
Vanillylmandelic acid, TMS
Vanilmandelic acid, TMS
Vanillylmandelic acid, 3tms derivative

Inchi: InChI=1S/C18H34O5Si3/c1-20-16-13-14(11-12-15(16)21-24(2,3)4)17(22-25(5,6)7)18(19)

InchiKey: QGOJNGYLGCWPKN-UHFFFAOYSA-N

Formula: C18H34O5Si3

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

Mol. weight [g/mol]: 414.72

CAS: 55268-66-1

Physical Properties

Property code	Value	Unit	Source
log10ws	1.58		Crippen Method
logp	5.180		Crippen Method
rinpol	1896.00		NIST Webbook
rinpol	1892.00		NIST Webbook
rinpol	1903.00		NIST Webbook
rinpol	1879.00		NIST Webbook
rinpol	1905.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1908.00		NIST Webbook
rinpol	1859.70		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1859.70		NIST Webbook
rinpol	1908.00		NIST Webbook

rinpol	1905.00	NIST Webbook
rinpol	1890.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55268661&Units=SI

Legend

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