Silanamine, N-[2-[3-methoxy-4-[(trimethylsilyl)oxy]phenyl]-N,1

Other names: Benzeneethanamine, 3-methoxy-N-methyl-N-(trimethylsilyl)-«beta»,4-bis[(trimethylsilyl)oxy]-
Benzenemethanol,4-hydroxy-3-methoxy-«alpha»-[(methylamino)methyl]-, tris(trimethylsilyl) deriv.
Metanephrine tri-TMS
Metanephrine, tris-TMS
Metanephrine, TMS
DL-Metanephrine, N,O,O'-(trimethylsilyl)-
Metanephrine, 3tms derivative

Inchi: InChI=1S/C19H39NO3Si3/c1-20(24(3,4)5)15-19(23-26(9,10)11)16-12-13-17(18(14-16)21

InchiKey: ZUOAVMHEWGXAQS-UHFFFAOYSA-N

Formula: C19H39NO3Si3

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

Mol. weight [g/mol]: 413.77

CAS: 56114-63-7

Physical Properties

Property code	Value	Unit	Source
log10ws	1.45		Crippen Method
logp	5.568		Crippen Method
rinpol	1950.00		NIST Webbook
rinpol	1938.00		NIST Webbook
rinpol	1907.10		NIST Webbook
rinpol	1907.10		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56114637&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices