3-Vanil-1,2-bis(trimethylsilyloxy)propane

Other names:	1,2-Propanediol, 3-(4-hydroxy-3-methoxyphenyl), tris-TMS
Inchi:	InChI=1S/C19H38O4Si3/c1-20-19-14-16(11-12-18(19)23-26(8,9)10)13-17(22-25(5,6)7)15
InchiKey:	BCALDHQTYOWJEV-UHFFFAOYSA-N
Formula:	C19H38O4Si3
SMILES:	COc1cc(CC(CO[Si](C)(C)C)O[Si](C)(C)C)ccc1O[Si](C)(C)C
Mol. weight [g/mol]:	414.76

Physical Properties

Property code	Value	Unit	Source
log10ws	1.28		Crippen Method
logp	5.523		Crippen Method
rinpol	1981.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U79085&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

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