3-VANIL-1,2-BIS(TRIMETHYLSILOXY)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]: 414.77

Physical Properties

Property code	Value	Unit	Source
ie	8.29	eV	Cheméo Relay (1.0)
logp	5.523		Crippen Method
rinpol	1981.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
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

ie: Ionization energy
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices