Benzenepropanol, 3-methoxy-4-(1-hydroxymethyl-2-(4-hydroxy-3-me tris-TMS

Inchi: InChI=1S/C29H50O5Si3/c1-30-28-20-23(13-12-18-32-35(3,4)5)14-16-26(28)25(22-33-36

InchiKey: GXGDWILLSUHMPB-UHFFFAOYSA-N

Formula: C29H50O5Si3

SMILES: COc1cc(CC(CO[Si](C)(C)C)c2ccc(CCCO[Si](C)(C)C)cc2OC)ccc1O[Si](C)(C)C

Mol. weight [g/mol]: 562.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.53		Crippen Method
logp	7.879		Crippen Method
rinpol	3014.00		NIST Webbook
rinpol	3014.00		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=R499486&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices