Octadecanoic acid, 9,10-dihydroxy, threo, methyl ester, DTBS

Inchi: InChI=1S/C27H54O4Si/c1-9-10-11-12-14-17-20-23-24(21-18-15-13-16-19-22-25(28)29-8
InchiKey: ZFMNFJGHBZLYCN-DNQXCXABSA-N
Formula: C27H54O4Si
SMILES: CCCCCCCCC1O[Si](C(C)(C)C)(C(C)(C)C)OC1CCCCCCCC(=O)OC
Mol. weight [g/mol]: 470.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.91		Crippen Method
logp	8.467		Crippen Method
rinpol	2690.00		NIST Webbook
rinpol	2690.00		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=R115465&Units=SI

Legend

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