11-Octadecenoic acid, 9,10,13-tris-hydroxy, TMS, methyl ester, # 2

Inchi: InChI=1S/C28H60O5Si3/c1-12-13-17-20-25(31-34(3,4)5)23-24-27(33-36(9,10)11)26(32-3

InchiKey: KSPFBLAYGBDSKW-VHXPQNKSSA-N

Formula: C28H60O5Si3

SMILES: CCCCCC(C=CC(O[Si](C)(C)C)C(CCCCCCCC(=O)OC)O[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]: 561.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.01		Crippen Method
logp	8.687		Crippen Method
rinpol	2545.00		NIST Webbook
rinpol	2545.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R398779&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