9,10,18-trihydroxyoctadec-12-enoic acid, TMSi ester TMSi ether

Inchi: InChI=1S/C30H66O5Si4/c1-36(2,3)32-27-23-19-14-13-16-20-24-28(33-37(4,5)6)29(34-38

InchiKey: RICDMDUPMDRSDE-SILNSSARSA-N

Formula: C30H66O5Si4

SMILES: C[Si](C)(C)OCCCCCC=CCC(O[Si](C)(C)C)C(CCCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]: 619.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.79		Crippen Method
logp	9.894		Crippen Method
rinpol	2848.00		NIST Webbook
rinpol	2848.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R423791&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices