10-Octadecenoic acid, 9,12,13-tris-hydroxy, TMS, methyl ester, # 1

Inchi: InChI=1S/C28H60O5Si3/c1-12-13-17-21-26(32-35(6,7)8)27(33-36(9,10)11)24-23-25(31-3

InchiKey: CXCODGVCNLKQLF-VHXPQNKSSA-N

Formula: C28H60O5Si3

SMILES: CCCCCC(O[Si](C)(C)C)C(C=CC(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	2526.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R398744&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

Latest version available from:

https://www.chemeo.com/cid/38-037-9/10-Octadecenoic-acid-9-12-13-tris-hydroxy-TMS-methyl-ester-1.pdf

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