

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

Inchi: InChI=1S/C28H60O5Si3/c1-30-28(29)24-20-16-13-15-19-23-27(33-36(8,9)10)26(32-35(5
InchiKey: WIZYORSJSLAYHG-JXAWBTAJSA-N
Formula: C28H60O5Si3
SMILES: COC(=O)CCCCCCCC(O[Si](C)(C)C)C(CC=CCCCCO[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 561.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.90		Crippen Method
logp	8.688		Crippen Method
rinpol	2743.00		NIST Webbook
rinpol	2743.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R423786&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/119-309-7/9-10-18-trihydroxyoctadec-12-enoic-acid-methyl-ester-TMSi-ether.pdf>

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