

11-Octadecenoic acid, 9,10,13-tris-hydroxy, TMS, methyl ester, # 3

Inchi: InChI=1S/C28H60O5Si3/c1-12-13-17-20-25(31-34(3,4)5)23-24-27(33-36(9,10)11)26(32-33)O[Si](C)(C)C
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	2550.00		NIST Webbook
rinpol	2550.00		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=R398784&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/45-403-4/11-Octadecenoic-acid-9-10-13-tris-hydroxy-TMS-methyl-ester-3.pdf>

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