

9,10,18-trihydroxyoctadecanoic acid, TMSi ester TMSi ether

Inchi: InChI=1S/C30H68O5Si4/c1-36(2,3)32-27-23-19-14-13-16-20-24-28(33-37(4,5)6)29(34-38)O[Si](C)(C)C
InchiKey: CBXDVZUGJCIRSA-UHFFFAOYSA-N
Formula: C30H68O5Si4
SMILES: C[Si](C)(C)OCCCCCCCC(O[Si](C)(C)C)C(CCCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 621.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.93		Crippen Method
logp	10.118		Crippen Method
rinpol	2878.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R423815&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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