Hexanoic acid, 2,3-bis-(OTMS) propyl ester («alpha»-glyceryl caproate)

Inchi: InChI=1S/C15H34O4Si2/c1-8-9-10-11-15(16)17-12-14(19-21(5,6)7)13-18-20(2,3)4/h14H

InchiKey: ZEUXMYZVZGHSML-UHFFFAOYSA-N

Formula: C15H34O4Si2

SMILES: CCCCCC(=O)OCC(CO[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]: 334.60

Physical Properties

Property code	Value	Unit	Source
log10ws	0.65		Crippen Method
logp	4.182		Crippen Method
rinpol	1668.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R517118&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