

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/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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