

Nonadecanoic acid, 1,3-bis-(OTMS) propyl ester («beta»-glyceryl nonadecanoate)

Inchi: InChI=1S/C28H60O4Si2/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-28(29)3
InchiKey: VCUOFTYKETZLHD-UHFFFAOYSA-N
Formula: C28H60O4Si2
SMILES: CCCCCCCCCCCCCCCCCC(=O)OC(CO[Si](C)(C)C)CO[Si](C)(C)C
Mol. weight [g/mol]: 516.94

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.79		Crippen Method
logp	9.253		Crippen Method
rinpol	2868.00		NIST Webbook
rinpol	2864.00		NIST Webbook
rinpol	2868.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R516982&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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