

Lauric acid, 2,3-bis(trimethylsiloxy)propyl ester

Other names:

Dodecanoic acid, 2,3-bis-(OTMS) propyl ester
2,3-bis-(OTMS)-«alpha»-glyceryl laurate
Dodecanoic acid, 2,3-bis-(OTMS) propyl ester («alpha»-glyceryl laurate)
Monolaurin, 2tms derivative

Inchi:

InChI=1S/C21H46O4Si2/c1-8-9-10-11-12-13-14-15-16-17-21(22)23-18-20(25-27(5,6)7)1

InchiKey:

FPYKFOLJVLTPBS-UHFFFAOYSA-N

Formula:

C₂₁H₄₆O₄Si₂

SMILES:

CCCCCCCCCCCC(=O)OCC(CO[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]:

418.76

CAS:

1116-65-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.86		Crippen Method
logp	6.522		Crippen Method
rinpol	2227.00		NIST Webbook
rinpol	2226.00		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=C1116650&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/23-049-2/Lauric-acid-2-3-bis-trimethylsiloxy-propyl-ester.pdf>

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