

cis, cis, cis-9, 12, 15-Octadecatrienoic acid, tert-butyldimethylsilyl ester

Other names:

Linolenic acid, TBDMS

«ALPHA»-linolenic acid, tbdms derivative

Inchi:

InChI=1S/C24H44O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(25)26-27(

InchiKey:

SLCZCEDSJXGESV-ORZIMQNZSA-N

Formula:

C24H44O2Si

SMILES:

CCC=CCC=CCC=CCCCCCCC(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]:

392.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.34		Crippen Method
logp	8.124		Crippen Method
rinpol	2470.10		NIST Webbook
rinpol	2472.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2468.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2468.00		NIST Webbook

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U333203&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/33-206-6/cis-cis-cis-9-12-15-Octadecatrienoic-acid-tert-butyltrimethylsilyl-ester.pdf>

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