

9,12-Octadecadienoic acid, tert-butyldimethylsilyl ester, (Z,Z)-

Other names:

Linoleic acid, DMTBS

Linoleic acid, TBDMS

cis-9,cis-12-Octadecadienoic acid, tert-butyldimethylsilyl ester

Inchi: InChI=1S/C24H46O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(25)26-27(

InchiKey: RDRZXODIXADGQF-HDXUUTQWSA-N

Formula: C24H46O2Si

SMILES: CCCCCC=CCC=CCCCCCCC(=O)O[Si](C)(C)C(C)C

Mol. weight [g/mol]: 394.71

CAS: 58160-91-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.49		Crippen Method
logp	8.348		Crippen Method
rinpol	2462.00		NIST Webbook
rinpol	2460.00		NIST Webbook
rinpol	2463.00		NIST Webbook
rinpol	2460.00		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=C58160911&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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