

9,12-Octadecadienoic acid (Z,Z)-, trimethylsilyl ester

Other names:

Linoleic acid trimethylsilyl ester
cis-9,cis-12-Octadecadienoic acid, trimethylsilyl ester
Linoleic acid, TMS
Trimethylsilyl cis,cis-9,12-octadecadienoate
(Z,Z)-9,12-Octadecadienoic acid, TMS
9,12-Octadecadienoic acid (9Z,12Z)-, trimethylsilyl ester
TMS cis,cis-9,12-octadecadienoate
9,12-Octadecadienoic acid (z,z)-, tms derivative

Inchi:

InChI=1S/C21H40O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-24(2,3)

InchiKey:

MXGBYOVWUYSJSN-UTJQPWESSA-N

Formula:

C21H40O2Si

SMILES:

CCCCC=CCC=CCCCCCCCC(=O)O[Si](C)(C)C

Mol. weight [g/mol]:

352.63

CAS:

56259-07-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.23		Crippen Method
logp	7.178		Crippen Method
rinpol	2212.00		NIST Webbook
rinpol	2208.50		NIST Webbook
rinpol	2214.00		NIST Webbook
rinpol	2210.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C56259075&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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.chemeo.com/cid/96-368-8/9-12-Octadecadienoic-acid-Z-Z-trimethylsilyl-ester.pdf>

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