

«alpha»-Linolenic acid, trimethylsilyl ester

Other names:	Trimethylsilyl (3Z,6Z,9Z)-3,6,9-octadecatrienoate «alpha»-Linolenic acid, TMS cis,cis,cis-9,12,15-Octadecatrienoic acid, trimethylsilyl ester Trimethylsilyl linolenate «ALPHA»-linolenic acid, tms derivative
Inchi:	InChI=1S/C21H38O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-24(2,3)
InchiKey:	DCFAEXKJEMZTKR-QNEBEIHSSA-N
Formula:	C21H38O2Si
SMILES:	CCC=CCC=CCC=CCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	350.61
CAS:	97844-13-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.09		Crippen Method
logp	6.954		Crippen Method
rinpol	2218.00		NIST Webbook
rinpol	2218.70		NIST Webbook
rinpol	2218.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97844138&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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