

cis-13,16-Docasadienoic acid, trimethylsilyl ester

Other names:	13,16-Docasadienoic acid, (z)-, tms derivative
Inchi:	InChI=1S/C25H48O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey:	GQGVFIYEJIDMDB-UTJQPWESSA-N
Formula:	C25H48O2Si
SMILES:	CCCCC=CCC=CCCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	408.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.91		Crippen Method
logp	8.738		Crippen Method
rinpola	2617.30		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333608&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
rinpola:	Non-polar retention indices

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<https://www.chemeo.com/cid/83-856-0/cis-13-16-Docasadienoic-acid-trimethylsilyl-ester.pdf>

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