

trans-13-Octadecenoic acid, trimethylsilyl ester

Other names:	13-Octadecenoic acid, (e)-, tms derivative
Inchi:	InChI=1S/C21H42O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-24(2,3)
InchiKey:	RNVCFFQAHYGLBB-CMDGGOBGSA-N
Formula:	C21H42O2Si
SMILES:	CCCCC=CCCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	354.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.38		Crippen Method
logp	7.402		Crippen Method
rinsol	2227.60		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333617&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.cheméo.com/cid/84-797-5/trans-13-Octadecenoic-acid-trimethylsilyl-ester.pdf>

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