

17-Octadecynoic acid, trimethylsilyl ester

Other names:	17-Octadecynoic acid, 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:	CCNBLZRYTUYUAX-UHFFFAOYSA-N
Formula:	C ₂₁ H ₄₀ O ₂ Si
SMILES:	C#CCCCCCCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	352.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.32		Crippen Method
logp	6.849		Crippen Method
rinpol	2256.80		NIST Webbook
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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=U333544&Units=SI

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/96-367-9/17-Octadecynoic-acid-trimethylsilyl-ester.pdf>

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