

# Isotetradecanoic acid, TMS

<b>Other names:</b>	Tridecanoic acid, 12-methyl, trimethylsilyl ester
<b>Inchi:</b>	InChI=1S/C17H36O2Si/c1-16(2)14-12-10-8-6-7-9-11-13-15-17(18)19-20(3,4)5/h16H,6-15H,17H,2H,3H,4H
<b>InchiKey:</b>	VDEGIVODSVYIDJ-UHFFFAOYSA-N
<b>Formula:</b>	C17H36O2Si
<b>SMILES:</b>	CC(C)CCCCCCCCC(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	300.55

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	5.921		Crippen Method
rinpol	1808.00		NIST Webbook
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## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R45340&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R45340&amp;Units=SI</a>

## Legend

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

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