

# cis, 6-Octadecenoic acid, trimethylsilyl ester

<b>Other names:</b>	Petroselinic acid, tms derivative
<b>Inchi:</b>	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)
<b>InchiKey:</b>	NEABEGUTEOTBEL-FOCLMDBBSA-N
<b>Formula:</b>	C21H42O2Si
<b>SMILES:</b>	CCCCCCCCCCCC=CCCCC(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	354.64
<b>CAS:</b>	96851-53-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.38		Crippen Method
logp	7.402		Crippen Method
rinpol	2209.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook

## 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=C96851535&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C96851535&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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