

# Citronellic acid, trimethylsilyl ester

<b>Other names:</b>	Citronellic acid, tms derivative
<b>Inchi:</b>	InChI=1S/C13H26O2Si/c1-11(2)8-7-9-12(3)10-13(14)15-16(4,5)6/h8,12H,7,9-10H2,1-6H
<b>InchiKey:</b>	NVBOIUPUPKAOBL-UHFFFAOYSA-N
<b>Formula:</b>	C13H26O2Si
<b>SMILES:</b>	CC(C)=CCCC(C)CC(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	242.43

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.79		Crippen Method
logp	4.137		Crippen Method
rinsol	1383.30		NIST Webbook
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## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U333631&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333631&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

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<https://www.chemeo.com/cid/117-881-4/Citronellic-acid-trimethylsilyl-ester.pdf>

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