

# 2-Keto-3-methylvaleric acid, TMS # 2

<b>Inchi:</b>	InChI=1S/C12H26O3Si2/c1-9-10(2)11(14-16(3,4)5)12(13)15-17(6,7)8/h9H2,1-8H3
<b>InchiKey:</b>	RHJGXCQRZWTGMA-UHFFFAOYSA-N
<b>Formula:</b>	C12H26O3Si2
<b>SMILES:</b>	CCC(C)=C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	274.50

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.75		Crippen Method
logp	3.900		Crippen Method
rinpol	1306.00		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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R400283&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R400283&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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