

# 2-Ketoisocaproic acid, trimethylsilyl ester

<b>Other names:</b>	4-Methyl-2-oxovaleric acid, trimethylsilyl ester 2-Ketoisocaproic acid, TMS ester 2-Ketoisocaproic acid, TMS # 1 2-Ketoisocaproic acid, tms derivative
<b>Inchi:</b>	InChI=1S/C9H18O3Si/c1-7(2)6-8(10)9(11)12-13(3,4)5/h7H,6H2,1-5H3
<b>InchiKey:</b>	MCPFMKJHOFUFFW-UHFFFAOYSA-N
<b>Formula:</b>	C9H18O3Si
<b>SMILES:</b>	CC(C)CC(=O)C(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	202.32
<b>CAS:</b>	74367-71-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.46		Crippen Method
logp	1.980		Crippen Method
rinsol	1115.20		NIST Webbook
rinsol	1129.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C74367718&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C74367718&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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