

# Butanoic acid, 3-methyl-, trimethylsilyl ester

<b>Other names:</b>	Isovaleric acid, trimethylsilyl ester 3-Methyl butanoic acid, TMS 3-Methylbutanoic acid, tms derivative
<b>Inchi:</b>	InChI=1S/C8H18O2Si/c1-7(2)6-8(9)10-11(3,4)5/h7H,6H2,1-5H3
<b>InchiKey:</b>	FEUVPJCEKKEDPZ-UHFFFAOYSA-N
<b>Formula:</b>	C8H18O2Si
<b>SMILES:</b>	CC(C)CC(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	174.31
<b>CAS:</b>	55557-13-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.16		Crippen Method
logp	2.411		Crippen Method
rinpol	932.00		NIST Webbook
rinpol	927.90		NIST Webbook
rinpol	978.00		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=C55557136&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55557136&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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