

# 2-Butenoic acid, 3-methyl-, trimethylsilyl ester

<b>Other names:</b>	Crotonic acid, 3-methyl-, trimethylsilyl ester Acrylic acid, 3,3-dimethyl-, trimethylsilyl ester Trimethylsilyl 3-methyl-2-butenate 3-Methyl-2-butenic acid, trimethylsilyl ester 3,3-Dimethylacrylic acid, trimethylsilyl ester Trimethylsilyl 3-methylbut-2-enoate Trimethylsilyl 3,3-dimethylacrylate 3,3-Dimethylacrylic acid, tms derivative
<b>Inchi:</b>	InChI=1S/C8H16O2Si/c1-7(2)6-8(9)10-11(3,4)5/h6H,1-5H3
<b>InchiKey:</b>	KNFZPFSOTLGZEE-UHFFFAOYSA-N
<b>Formula:</b>	C8H16O2Si
<b>SMILES:</b>	CC(C)=CC(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	172.30
<b>CAS:</b>	25436-25-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.06		Crippen Method
logp	2.331		Crippen Method
rinpol	1015.00		NIST Webbook
rinpol	1002.70		NIST Webbook
rinpol	1007.20		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=C25436253&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C25436253&amp;Units=SI</a>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**rinpol:** Non-polar retention indices

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