

# 3-Butenoic acid, trimethylsilyl ester

<b>Other names:</b>	3-Butenoic acid, tms derivative
<b>Inchi:</b>	InChI=1S/C7H14O2Si/c1-5-6-7(8)9-10(2,3)4/h5H,1,6H2,2-4H3
<b>InchiKey:</b>	NJLWVYLLRXIFHK-UHFFFAOYSA-N
<b>Formula:</b>	C7H14O2Si
<b>SMILES:</b>	C=CCC(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	158.27

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.48		Crippen Method
logp	1.941		Crippen Method
rinpol	874.10		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=U333860&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333860&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

Latest version available from:

<https://www.chemeo.com/cid/51-316-4/3-Butenoic-acid-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-28 07:06:46.472576022 +0000 UTC m=+16577255.393153337.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.