

# Butanedioic acid, methylene-, bis(trimethylsilyl) ester

<b>Other names:</b>	Itaconic acid (2TMS) Itaconic acid, di-TMS Itaconic acid, bis-TMS ester Mesaconic acid, di-TMS Itaconic acid (tms) Mesaconic acid, TMS Itaconic acid, 2tms derivative
<b>Inchi:</b>	InChI=1S/C11H22O4Si2/c1-9(11(13)15-17(5,6)7)8-10(12)14-16(2,3)4/h1,8H2,2-7H3
<b>InchiKey:</b>	IYEWOPPVIQNFQO-UHFFFAOYSA-N
<b>Formula:</b>	C11H22O4Si2
<b>SMILES:</b>	C=C(CC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	274.46
<b>CAS:</b>	55494-04-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	1.89		Crippen Method
logp	2.689		Crippen Method
rinpol	1400.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1419.00		NIST Webbook

## Sources

<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=C55494047&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55494047&amp;Units=SI</a>
<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>

## Legend

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

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