

# trans-3-Hexenedioic acid, bis(trimethylsilyl) ester

<b>Other names:</b>	trans-3-Hydromuconic acid, TMS trans-3-Hexenedioic acid, TMS trans-3-Dihydromuconic acid, TMS 3-Hexenedioic acid, (e)-, 2tms derivative
<b>Inchi:</b>	InChI=1S/C12H24O4Si2/c1-17(2,3)15-11(13)9-7-8-10-12(14)16-18(4,5)6/h7-8H,9-10H2,
<b>InchiKey:</b>	ZHDWBZJDVFQQO-BQYQJAHWSA-N
<b>Formula:</b>	C12H24O4Si2
<b>SMILES:</b>	C[Si](C)(C)OC(=O)CC=CCC(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	288.49

## Physical Properties

Property code	Value	Unit	Source
log10ws	1.47		Crippen Method
logp	3.079		Crippen Method
rinpol	1506.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1503.00		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=U78954&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U78954&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

<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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