

# 2-Hexenedioic acid, TMS

<b>Other names:</b>	2-Hexenedioic acid, diTMS
<b>Inchi:</b>	InChI=1S/C12H24O4Si2/c1-17(2,3)15-11(13)9-7-8-10-12(14)16-18(4,5)6/h7,9H,8,10H2,1
<b>InchiKey:</b>	BVXJLSYCPJDQEM-VQHVLOKHSA-N
<b>Formula:</b>	C12H24O4Si2
<b>SMILES:</b>	C[Si](C)(C)OC(=O)C=CCCC(=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
rinpola	1522.00		NIST Webbook
rinpola	1522.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R493562&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R493562&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>rinpola:</b>	Non-polar retention indices

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<https://www.chemeo.com/cid/71-771-7/2-Hexenedioic-acid-TMS.pdf>

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