

# 2-Deoxy-3-C-(hydroxymethyl)tetraric acid, TMS

<b>Inchi:</b>	InChI=1S/C17H40O6Si4/c1-24(2,3)20-14-17(23-27(10,11)12,16(19)22-26(7,8)9)13-15(18)
<b>InchiKey:</b>	CUGMQWBISPXASF-QGZVFWFLSA-N
<b>Formula:</b>	C17H40O6Si4
<b>SMILES:</b>	C[Si](C)(C)OCC(CC(=O)O[Si](C)(C)C)(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	452.84

## Physical Properties

Property code	Value	Unit	Source
log10ws	4.85		Crippen Method
logp	4.574		Crippen Method
rinpol	1714.00		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=R100899&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R100899&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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