

# 1,4:3,6-Dianhydromannitol, TMS

<b>Inchi:</b>	InChI=1S/C12H26O4Si2/c1-17(2,3)15-9-7-13-12-10(8-14-11(9)12)16-18(4,5)6/h9-12H,7-
<b>InchiKey:</b>	LJFXZWTUMDMOLO-NNYUYHANSA-N
<b>Formula:</b>	C12H26O4Si2
<b>SMILES:</b>	C[Si](C)(C)OC1COC2C(O[Si](C)(C)C)COC12
<b>Mol. weight [g/mol]:</b>	290.50

## Physical Properties

Property code	Value	Unit	Source
log10ws	2.47		Crippen Method
logp	2.224		Crippen Method
rinpol	1537.00		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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R74131&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R74131&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

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