

# 1,4-Anhydro-3-deoxypentitol-2-carboxylic acid, TMS

<b>Inchi:</b>	InChI=1S/C12H26O4Si2/c1-17(2,3)15-9-11-7-10(8-14-11)12(13)16-18(4,5)6/h10-11H,7-9
<b>InchiKey:</b>	IEVXRVGHUBGOBQ-UHFFFAOYSA-N
<b>Formula:</b>	C12H26O4Si2
<b>SMILES:</b>	C[Si](C)(C)OCC1CC(C(=O)O[Si](C)(C)C)CO1
<b>Mol. weight [g/mol]:</b>	290.50

## Physical Properties

Property code	Value	Unit	Source
log10ws	2.25		Crippen Method
logp	2.621		Crippen Method
rinpol	1652.00		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=R100686&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R100686&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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