

# 3A,21-Dihydroxy-5B-pregnan-11,20-dione, MO TMS

<b>Other names:</b>	5B-Pregnan-3A,21-diol-11,20-dione, MO TMS 5«beta»-Pregnane-3«alpha», 21-diol-11, 20-dione (THA), MO TMS
<b>Inchi:</b>	InChI=1S/C29H54N2O4Si2/c1-28-16-15-21(35-37(8,9)10)17-20(28)11-12-22-23-13-14-2
<b>InchiKey:</b>	DQHCAIQGKVDNTB-QPIHRGTRSA-N
<b>Formula:</b>	C29H54N2O4Si2
<b>SMILES:</b>	CON=C(CO[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(=NOC)CC12C
<b>Mol. weight [g/mol]:</b>	550.92

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Crippen Method
logp	7.332		Crippen Method
rinpol	2991.00		NIST Webbook
rinpol	2990.00		NIST Webbook
rinpol	2978.00		NIST Webbook
rinpol	2971.00		NIST Webbook
rinpol	2989.00		NIST Webbook
rinpol	2988.00		NIST Webbook
rinpol	2979.00		NIST Webbook
rinpol	3002.00		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=R97595&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R97595&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

**rinpol:** Non-polar retention indices

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