

# 4-Pregnen-11-«beta»,20-«beta»-diol-3-one, MO-TMS

<b>Inchi:</b>	InChI=1S/C28H51NO3Si2/c1-19(31-33(5,6)7)23-13-14-24-22-12-11-20-17-21(29-30-4)15
<b>InchiKey:</b>	POLSCKPVKDCQEJ-DGEIVTRFSA-N
<b>Formula:</b>	C28H51NO3Si2
<b>SMILES:</b>	CON=C1C=C2CCC3C(C(O[Si](C)(C)C)CC4(C)C(C(C)O[Si](C)(C)C)CCC34)C2(C)CC1
<b>Mol. weight [g/mol]:</b>	505.88

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	7.638		Crippen Method
rinpol	3084.00		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=R486143&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R486143&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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