

# 5-«alpha»-Pregnan-20-«beta»-ol-3,11-dione, MO-TMS

<b>Inchi:</b>	InChI=1S/C26H46N2O3Si/c1-17(31-32(6,7)8)21-11-12-22-20-10-9-18-15-19(27-29-4)13-
<b>InchiKey:</b>	NAHQLWIRZFYOOZ-ZZFWAJHVSA-N
<b>Formula:</b>	C26H46N2O3Si
<b>SMILES:</b>	CON=C1CCC2(C)C(CCC3C4CCC(C(C)O[Si](C)(C)C)C4(C)CC(=NOC)C32)C1
<b>Mol. weight [g/mol]:</b>	462.74

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.33		Crippen Method
logp	6.500		Crippen Method
rinpol	2956.00		NIST Webbook
rinpol	2956.00		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=R486485&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R486485&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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