

# 5«beta»-Pregnane-3«alpha»,20«alpha»-diol, (3-O)-TBDMSi

Inchi:	InChI=1S/C27H50O2Si/c1-18(28)22-11-12-23-21-10-9-19-17-20(29-30(7,8)25(2,3)4)13-1
InchiKey:	BGTQQFMWJQOKOI-TXUGEVFPSA-N
Formula:	C27H50O2Si
SMILES:	CC(O)C1CCC2C3CCC4CC(O[Si](C)(C)C(C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	434.77

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.64		Crippen Method
logp	7.417		Crippen Method
rinpol	2908.00		NIST Webbook
rinpol	2945.00		NIST Webbook
rinpol	2908.00		NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R144319&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R144319&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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