

# 5-Pregnene-3«beta»,20«alpha»,21-triol, tris-TMS

Inchi:	InChI=1S/C30H58O3Si3/c1-29-18-16-23(32-35(6,7)8)20-22(29)12-13-24-25-14-15-27(30)
InchiKey:	RBSXFFWTNZTHKA-LWZJXHPASA-N
Formula:	C30H58O3Si3
SMILES:	CC12CCC(O[Si](C)(C)C)CC1=CCC1C2CCC2(C)C(C(CO[Si](C)(C)C)O[Si](C)(C)C)CCC1
Mol. weight [g/mol]:	551.04

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	8.857		Crippen Method
rinpol	3090.00		NIST Webbook
rinpol	3090.00		NIST Webbook

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R528871&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R528871&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>
Crippen Method:	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## Legend

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

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