

# 3A,11B,17A,21-Tetrahydroxy-5A-pregnan-20-one, MO TMS

Other name:  
MO TMS  
Inchi:

5«alpha»-Pregnane-3«alpha», 11«beta», 17«alpha», 21-tetrol-20-one (Allo-THF),  
MO TMS  
InChI=1S/C34H69NO5Si4/c1-32-20-18-26(38-42(7,8)9)22-25(32)16-17-27-28-19-21-34(4

InchiKey:

WZZDCZPDFSSOIG-XIXNWTBSSA-N

Formula:

C34H69NO5Si4

SMILES:

CON=C(CO[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C

Mol. weight [g/mol]:

684.26

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.31		Crippen Method
logp	9.523		Crippen Method
rinpol	3043.00		NIST Webbook
rinpol	3036.00		NIST Webbook
rinpol	3049.00		NIST Webbook
rinpol	3049.00		NIST Webbook
rinpol	3036.00		NIST Webbook
rinpol	3051.00		NIST Webbook
rinpol	3050.00		NIST Webbook

## Sources

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R486014&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

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

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