

# 5«alpha»-Pregnane-3«alpha»,11«beta»,20«alpha»

**EO-TMS**

InChIKey:

InChI=1S/C29H58O3Si3/c1-20(30-33(3,4)5)25-16-17-26-24-14-12-21-18-22(31-34(6,7)8)

MGCSXZOEJYDJ-ZNTRDUKVSA-N

Formula:

C<sub>29</sub>H<sub>58</sub>O<sub>3</sub>Si<sub>3</sub>

SMILES:

CC(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4C3C(O[Si](C)(C)C)CC12C

Mol. weight [g/mol]:

539.03

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.60		Crippen Method
logp	8.545		Crippen Method
rinpol	2913.00		NIST Webbook
rinpol	2918.00		NIST Webbook
rinpol	2911.00		NIST Webbook
rinpol	2913.00		NIST Webbook

## Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R526944&Units=SI>

## Legend

**log10ws:**

Log10 of Water solubility in mol/l

**logp:**

Octanol/Water partition coefficient

**rinpol:**

Non-polar retention indices

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