

# 5-«beta»-Pregnan-11-«beta»,20-«beta»-diol-3-one

## MO-TMS

InchiKey:

InChI=1S/C28H53NO3Si2/c1-19(31-33(5,6)7)23-13-14-24-22-12-11-20-17-21(29-30-4)15

Formula:

C28H53NO3Si2

SMILES:

CON=C1CCC2(C)C(CCC3C4CCC(C(C)O[Si](C)(C)C)C4(C)CC(O[Si](C)(C)C)C32)C1

Mol. weight [g/mol]:

507.90

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	7.718		Crippen Method
rinpol	2950.00		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=R486767&Units=SI>

Crippen Method:

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

## Legend

**log10ws:**

Log10 of Water solubility in mol/l

**logp:**

Octanol/Water partition coefficient

**rinpol:**

Non-polar retention indices

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<https://www.chemeo.com/cid/58-702-8/5-beta-Pregnan-11-beta-20-beta-diol-3-one-MO-TMS.pdf>

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