

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

## MO-TMS

InchiKey:

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

Formula:

C28H53NO3Si2

SMILES:

CON=C(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)CC12C

Mol. weight [g/mol]:

507.90

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	7.718		Crippen Method
rinpol	2972.00		NIST Webbook

## Sources

Crippen Method:

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

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=R486658&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/21-958-5/5-alpha-Pregnan-3-beta-11-beta-diol-20-one-MO-TMS.pdf>

Generated by Cheméo on 2024-04-28 20:26:03.077778546 +0000 UTC m=+16625211.998355861.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.