

# Pregnan-20-one, 3,11,21-tris[(trimethylsilyl)oxy]-, (3«alpha»,5«beta»,11«beta»)-

Other names: 3,11,21-Tris[(trimethylsilyl)oxy]pregnan-20-one-, (3«alpha»,5«beta»,11«beta»)-  
Tetrahydrocorticosterone, (3 TMS)

Tetrahydrocorticosterone, tris-TMS

Tetrahydrocorticosterone, TMS

**Inchi:** InChI=1S/C30H58O4Si3/c1-29-17-16-22(33-36(6,7)8)18-21(29)12-13-23-24-14-15-25(26)  
**InchiKey:** UNLCXDYGUPZCQD-JOQFUENTSA-N  
**Formula:** C30H58O4Si3  
**SMILES:** CC12CC(O[Si](C)(C)C)C3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CCC2C(=O)CO[Si](C)(C)C  
**Mol. weight [g/mol]:** 567.04  
**CAS:** 56196-42-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.19		Crippen Method
logp	8.116		Crippen Method
rinsol	3177.00		NIST Webbook
rinsol	3190.00		NIST Webbook
rinsol	3156.00		NIST Webbook
rinsol	3177.00		NIST Webbook

## Sources

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

**Crippen Method:** [https://www.chemed.com/doc/models/crippen\\_log10ws](https://www.chemed.com/doc/models/crippen_log10ws)

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C56196420&Units=SI>

## Legend

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

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