

# 5«beta»-Pregnane-3«alpha», 11«beta», 21-triol-20-one (THB), MO TMS

**Inchi:** InChI=1S/C31H61NO4Si3/c1-30-18-17-23(35-38(7,8)9)19-22(30)13-14-24-25-15-16-26(27,28)29  
**InchiKey:** LTUTXXUPIPZWMI-YIHWBZEHSA-N  
**Formula:** C31H61NO4Si3  
**SMILES:** CON=C(CO[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)C1  
**Mol. weight [g/mol]:** 596.08

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.57		Crippen Method
logp	8.549		Crippen Method
rinpol	3016.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R250489&Units=SI>  
**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)

## Legend

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

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