

# 5«beta»-pregnane-3«alpha»,17«alpha»,20«beta»-triol, (3,17,20-O)-triTMSi

**Other names:** 5«beta»-pregnane-3«alpha»,17«alpha»,20«alpha»-triol, (3,17,20-O)-triTMSi  
**Inchi:** InChI=1S/C30H60O3Si3/c1-22(31-34(4,5)6)30(33-36(10,11)12)20-17-27-25-14-13-23-21

**InchiKey:** KFUWLVZCEDFJIK-CBBCAGDGSA-N

**Formula:** C30H60O3Si3

**SMILES:** CC(O[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21O

**Mol. weight [g/mol]:** 553.05

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.26		Crippen Method
logp	9.079		Crippen Method
rinpola	2811.00		NIST Webbook
rinpola	2845.00		NIST Webbook
rinpola	2765.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R93220&Units=SI>

**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)

## Legend

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

**logp:** Octanol/Water partition coefficient

**rinpola:** Non-polar retention indices

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