# 5«beta»-pregnane-3«alpha»,17,20«alpha»-triol, MO-TMS

**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-AEXGWUNBSA-N

**Formula:** C30H60O3Si3

**SMILES:** CC(O[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C

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

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -2.26 | | Crippen Method |
| logp | 9.079 | | Crippen Method |
| rinpol | 2889.00 | | NIST Webbook |
| rinpol | 2889.00 | | NIST Webbook |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R488298&Units=SI

## Legend

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

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices