

# 5«beta»-Pregnane-3«alpha»,17«alpha»,20«alpha» (3,17-O)-diTMTBSi, (20-O)-TMSi

InChI: InChI=1S/C40H76O3Si3/c1-30(42-45)11(12)40(43-46(36(2,3)4)27-15-16-28-46)26-21  
InChIKey: VZQVHBDHUGHRQR-YMIBEPHVSA-N

Formula: C<sub>40</sub>H<sub>76</sub>O<sub>3</sub>Si<sub>3</sub>  
SMILES: CC(O[Si](C)(C)C)C1(O[Si]2(C(C)(C)C)CCCC2)CCC2C3CCC4CC(OC5([Si](C)(C)C)CCC  
Mol. weight [g/mol]: 689.29

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -5.85   |      | Crippen Method |
| logp          | 12.139  |      | Crippen Method |
| rinpol        | 3896.00 |      | 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=R385981&Units=SI>

## Legend

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

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