

# PGD1, EO-TMS, isomer # 1

**Inchi:** InChI=1S/C31H63NO5Si3/c1-12-14-17-20-26(35-38(3,4)5)23-24-27-28(21-18-15-16-19-20)/1-2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31  
**InchiKey:** KZUHVQWLOMUWAS-BPXHILEUSA-N  
**Formula:** C31H63NO5Si3  
**SMILES:** CCCCCC(C=CC1C(=NOCC)CC(O[Si](C)(C)C)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C  
**Mol. weight [g/mol]:** 614.09

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.72   |      | Crippen Method |
| logp          | 9.310   |      | Crippen Method |
| rinpol        | 2766.00 |      | NIST Webbook   |
| rinpol        | 2766.00 |      | NIST Webbook   |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581738&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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