

# PGD1, MO-TMS, isomer # 2

**Inchi:** InChI=1S/C30H61NO5Si3/c1-12-13-16-19-25(34-37(3,4)5)22-23-26-27(29(35-38(6,7)8)2  
**InchiKey:** HEQOKIBNBHDCGP-CGXNDPOCSA-N  
**Formula:** C30H61NO5Si3  
**SMILES:** CCCCCC(C=CC1C(=NOC)CC(O[Si](C)(C)C)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)  
**Mol. weight [g/mol]:** 600.07

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.30   |      | Crippen Method |
| logp          | 8.920   |      | Crippen Method |
| rinpol        | 2761.00 |      | NIST Webbook   |
| rinpol        | 2761.00 |      | NIST Webbook   |

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581763&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

Latest version available from:

<https://www.cheméo.com/cid/122-984-4/PGD1-MO-TMS-isomer-2.pdf>

Generated by Cheméo on 2024-04-30 07:02:39.488246783 +0000 UTC m=+16749808.408824102.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.