

# 15(S)-15-Methyl-PGA2, BO-TMS, isomer # 1

**Inchi:** InChI=1S/C31H57NO4Si2/c1-10-12-18-24-31(3,36-38(7,8)9)25-23-27-21-22-29(32-34-26)  
**InchiKey:** PFHNSQOPBICNCF-CWZPGBDYSA-N  
**Formula:** C31H57NO4Si2  
**SMILES:** CCCCC(C)(C=CC1C=CC(=NOCCCC)C1CC=CCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C  
**Mol. weight [g/mol]:** 563.96

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -5.18   |      | Crippen Method |
| logp          | 9.203   |      | Crippen Method |
| rinpol        | 2762.00 |      | NIST Webbook   |
| rinpol        | 2762.00 |      | 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=R581263&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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