

# PGA1, EO-TMS, isomer # 2

**Inchi:** InChI=1S/C28H53NO4Si2/c1-9-11-14-17-25(32-34(3,4)5)22-20-24-21-23-27(29-31-10-2)  
**InchiKey:** AEJQJLKSHLXDED-WDMRMWGLSA-N  
**Formula:** C28H53NO4Si2  
**SMILES:** CCCCCC(C=CC1C=CC(=NOCC)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C  
**Mol. weight [g/mol]:** 523.90

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -4.07   |      | Crippen Method |
| logp          | 8.256   |      | Crippen Method |
| rinpol        | 2652.00 |      | NIST Webbook   |
| rinpol        | 2652.00 |      | NIST Webbook   |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581565&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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<https://www.chemeo.com/cid/28-310-6/PGA1-EO-TMS-isomer-2.pdf>

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