

# PGE2, EO-TMS, isomer # 1

**Inchi:** InChI=1S/C31H61NO5Si3/c1-12-14-17-20-26(35-38(3,4)5)23-24-28-27(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:** AJOVLGPPFOBIEN-XECDJUQESA-N  
**Formula:** C31H61NO5Si3  
**SMILES:** CCCCCC(C=CC1C(O[Si](C)(C)C)CC(=NOCC)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C)O[Si](C)(C)C  
**Mol. weight [g/mol]:** 612.08

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	9.086		Crippen Method
rinpol	2726.00		NIST Webbook
rinpol	2726.00		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=R581916&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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