

# PGE2, BO-TMS, isomer # 1

**Inchi:** InChI=1S/C33H65NO5Si3/c1-12-14-18-21-28(37-40(3,4)5)24-25-30-29(22-19-16-17-20-23)31-32-33  
**InchiKey:** KNYXDDWQYFOER-BTZWMAIRSA-N  
**Formula:** C33H65NO5Si3  
**SMILES:** CCCCCC(C=CC1C(O[Si](C)(C)C)CC(=NOCCCC)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C  
**Mol. weight [g/mol]:** 640.13

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	9.867		Crippen Method
rinpol	2887.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581892&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

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