

# PGE1, MO-TMS, isomer # 1

**Inchi:** InChI=1S/C30H61NO5Si3/c1-12-13-16-19-25(34-37(3,4)5)22-23-27-26(28(31-33-2)24-29)  
**InchiKey:** NYKPCVVFAUFGKOP-RBSDKKBGESA-N  
**Formula:** C30H61NO5Si3  
**SMILES:** CCCCCC(C=CC1C(O[Si](C)(C)C)CC(=NOC)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(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	2703.00		NIST Webbook
rinpol	2703.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581872&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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