

# 15-Keto-PGA1A, EO-TMS, isomer # 1

**Inchi:** InChI=1S/C27H48N2O4Si/c1-7-10-13-16-24(28-31-8-2)21-19-23-20-22-26(29-32-9-3)25  
**InchiKey:** RJRAIJKIHSVOZ-JSNAYEGTSA-N  
**Formula:** C27H48N2O4Si  
**SMILES:** CCCCCC(C=CC1C=CC(=NOCC)C1CCCCCCC(=O)O[Si](C)(C)C)=NOCC  
**Mol. weight [g/mol]:** 492.77

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.64		Crippen Method
logp	7.429		Crippen Method
rinpol	2780.00		NIST Webbook
rinpol	2780.00		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=R581050&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/11-017-0/15-Keto-PGA1A-EO-TMS-isomer-1.pdf>

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