

# PGA1, BO-TMS, isomer # 2

**Inchi:** InChI=1S/C30H57NO4Si2/c1-9-11-15-18-27(34-36(3,4)5)23-21-26-22-24-29(31-33-25-12)  
**InchiKey:** YOJSASACMPRYDX-CSHHMKSISA-N  
**Formula:** C30H57NO4Si2  
**SMILES:** CCCCCC(C=CC1C=CC(=NOCCCC)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C  
**Mol. weight [g/mol]:** 551.95

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.90		Crippen Method
logp	9.037		Crippen Method
rinpol	2845.00		NIST Webbook
rinpol	2845.00		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=R581545&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/113-557-8/PGA1-BO-TMS-isomer-2.pdf>

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