

# PGA2, BO-TMS, isomer # 1

**Inchi:** InChI=1S/C30H55NO4Si2/c1-9-11-15-18-27(34-36(3,4)5)23-21-26-22-24-29(31-33-25-12)  
**InchiKey:** JLXZPPNHDUATET-VHBSRNPFSAN  
**Formula:** C30H55NO4Si2  
**SMILES:** CCCCC(C=CC1C=CC(=NOCCCC)C1CC=CCCC(=O)O[Si](C)(C)O[Si](C)(C)C  
**Mol. weight [g/mol]:** 549.93

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	8.813		Crippen Method
rinpol	2745.00		NIST Webbook
rinpol	2745.00		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=R581590&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**rinpol:** Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/121-069-1/PGA2-BO-TMS-isomer-1.pdf>

Generated by Cheméo on 2024-04-28 10:11:23.811373847 +0000 UTC m=+16588332.731951159.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.