

# PGA2, BO-TMS, isomer # 2

**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:** CCCCCC(C=CC1C=CC(=NOCCCC)C1CC=CCCCC(=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
rinsol	2826.00		NIST Webbook
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## 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=R581609&Units=SI>

## Legend

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

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<https://www.chemeo.com/cid/113-582-0/PGA2-BO-TMS-isomer-2.pdf>

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