

# Allopregnenediol TMS

**Inchi:** InChI=1S/C28H54O2Si2/c1-10-26(30-32(7,8)9)25-14-13-23-22-12-11-20-19-21(29-31(4,5)6)3  
**InchiKey:** FFOITQMJIMFGSD-BBEQGNITSA-N  
**Formula:** C28H54O2Si2  
**SMILES:** CCC(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C  
**Mol. weight [g/mol]:** 478.90

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	8.495		Crippen Method
rinpol	2783.00		NIST Webbook
rinpol	2796.00		NIST Webbook

## Sources

**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=R97620&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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/53-561-0/Allopregnenediol-TMS.pdf>

Generated by Cheméo on 2024-04-26 05:21:18.362405563 +0000 UTC m=+16398127.282982879.

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