

# Pregnanediol MO 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)33-27-24-28-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100  
**InchiKey:** FFOITQMJIMFGSD-SAGLKEOOSA-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	2779.00		NIST Webbook
rinpol	2790.00		NIST Webbook
rinpol	2802.00		NIST Webbook
rinpol	2802.00		NIST Webbook
rinpol	2779.00		NIST Webbook
rinpol	2758.00		NIST Webbook
rinpol	2785.00		NIST Webbook
rinpol	2786.00		NIST Webbook
rinpol	2764.00		NIST Webbook
rinpol	2799.00		NIST Webbook
rinpol	2799.00		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=R97666&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices

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