

# allo-Tetrahydrocortosterone, TMSO-TMS # 2

**Inchi:** InChI=1S/C33H67NO4Si4/c1-32-20-19-25(36-40(6,7)8)21-24(32)15-16-26-27-17-18-28(29,30,31)33  
**InchiKey:** PPNLCQXZSCQULC-BSVZLILSSA-N  
**Formula:** C33H67NO4Si4  
**SMILES:** CC12CC(O[Si](C)(C)C)C3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CCC2C(CO[Si](C)(C)C)C2  
**Mol. weight [g/mol]:** 654.23

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.45		Crippen Method
logp	9.754		Crippen Method
rinpol	3100.00		NIST Webbook
rinpol	3100.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527501&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

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

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