

# Ergosterol TMS

**Inchi:** InChI=1S/C31H52OSi/c1-21(2)22(3)10-11-23(4)27-14-15-28-26-13-12-24-20-25(32-33(7)  
**InchiKey:** OPWXUPLJCANTIU-WSYNUCCGSA-N  
**Formula:** C31H52OSi  
**SMILES:** CC(C)C(C)C=CC(C)C1CCC2C3=CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C  
**Mol. weight [g/mol]:** 468.83

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.26		Crippen Method
logp	9.190		Crippen Method
rinpol	3191.00		NIST Webbook
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rinpol	3191.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R500219&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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