

# 11-Ketoetiocholanolone MO TMS

**Other names:** 11-oxoetiocholanolone, MO TMS  
**Inchi:** InChI=1S/C24H42N2O3Si/c1-23-13-12-17(29-30(5,6)7)14-16(23)8-9-18-19-10-11-21(26-27)22-24  
**InchiKey:** CZAVIQKBQLKTIH-OUBBBIISA-N  
**Formula:** C<sub>24</sub>H<sub>42</sub>N<sub>2</sub>O<sub>3</sub>Si  
**SMILES:** CON=C1CC2(C)C(=NOC)CCC2C2CCC3CC(O[Si](C)(C)C)CCC3(C)C12  
**Mol. weight [g/mol]:** 434.69

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.73		Crippen Method
logp	5.864		Crippen Method
rinpol	2627.00		NIST Webbook
rinpol	2630.00		NIST Webbook
rinpol	2610.00		NIST Webbook
rinpol	2632.00		NIST Webbook
rinpol	2636.00		NIST Webbook
rinpol	2656.00		NIST Webbook
rinpol	2646.00		NIST Webbook
rinpol	2601.00		NIST Webbook
rinpol	2601.00		NIST Webbook
rinpol	2627.00		NIST Webbook
rinpol	2610.00		NIST Webbook
rinpol	2656.00		NIST Webbook
rinpol	2610.00		NIST Webbook

## 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=R92666&Units=SI>

# Legend

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

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