

# «alpha»-Estradiol, bis(trimethylsilyl) ether

**Other names:** «alpha»-Estradiol, TMS  
17A-Oestradiol, TMS

**Inchi:** InChI=1S/C24H40O2Si2/c1-24-15-14-20-19-11-9-18(25-27(2,3)4)16-17(19)8-10-21(20)2

**InchiKey:** WJUROLKZHWTVGC-NEUFXUDDSA-N

**Formula:** C<sub>24</sub>H<sub>40</sub>O<sub>2</sub>Si<sub>2</sub>

**SMILES:** CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CCC2O[Si](C)(C)C

**Mol. weight [g/mol]:** 416.74

**CAS:** 33283-14-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.86		Crippen Method
logp	6.976		Crippen Method
rinpol	2595.00		NIST Webbook
rinpol	2656.40		NIST Webbook
rinpol	2595.00		NIST Webbook
rinpol	2656.40		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=C33283146&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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