

# Silane, [(16«beta»,17«alpha»)-estra-1,3,5(10)-triene-3,16,

Other names:

Silane,  
[(16«beta»,17«alpha»)-estra-1,3,5(10)-triene-3,16,17-triyl]tris(oxy)tris(trimethyl-  
3,16«beta»,17«alpha»-Trihydroxy-1,3,5(10)-estratriene 3,16,17-tris

16-Epiestriol, 3,16,17-tris(trimethylsilyl) ether

16«BETA»,17«alpha»-estriol, 3tms derivative

**Inchi:** InChI=1S/C27H48O3Si3/c1-27-16-15-22-21-14-12-20(28-31(2,3)4)17-19(21)11-13-23(22

**InchiKey:** MCKRDIGCTGOZEH-UHFFFAOYSA-N

**Formula:** C27H48O3Si3

**SMILES:** CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CC(O[Si](C)(C)C)C2O[Si](C)(C)C

**Mol. weight [g/mol]:** 504.92

**CAS:** 57305-22-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.37		Crippen Method
logp	7.806		Crippen Method
rmpol	2929.60		NIST Webbook
rmpol	2890.00		NIST Webbook
rmpol	2899.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C57305223&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemo.com/doc/models/crippen\\_log10ws](https://www.chemo.com/doc/models/crippen_log10ws)

## Legend

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

**logp:** Octanol/Water partition coefficient

**rmpol:** Non-polar retention indices

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