

# Trimethylsilylestrone

**Other names:**

Estra-1,3,5(10)-trien-17-one, 3-[(trimethylsilyl)oxy]-  
Estra-1,3,5(10)-trien-17-one, 3-(trimethylsiloxy)-  
Estrone trimethylsilyl ether  
Estrone-TMS ether  
Oestrone, TMS  
Estrone, tms derivative

**Inchi:**

InChI=1S/C21H30O2Si/c1-21-12-11-17-16-8-6-15(23-24(2,3)4)13-14(16)5-7-18(17)19(20)

**InchiKey:**

FRJOURBWXHQBBER-UHFFFAOYSA-N

**Formula:**

C<sub>21</sub>H<sub>30</sub>O<sub>2</sub>Si

**SMILES:**

CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CCC2=O

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

342.55

**CAS:**

1839-54-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.64		Crippen Method
logp	5.325		Crippen Method
rinpol	2532.00		NIST Webbook
rinpol	2535.00		NIST Webbook
rinpol	2532.00		NIST Webbook
rinpol	2535.00		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=C1839549&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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