

# 17«alpha»-Ethinylestradiol, 3-(tert-butyl dimethylsilyl) ether

**Other names:** Ethinyl estradiol, tbdms derivative  
**Inchi:** InChI=1S/C26H38O2Si/c1-8-26(27)16-14-23-22-11-9-18-17-19(28-29(6,7)24(2,3)4)10-12  
**InchiKey:** CSZIVCGZGDDUNR-UHFFFAOYSA-N  
**Formula:** C<sub>26</sub>H<sub>38</sub>O<sub>2</sub>Si  
**SMILES:** C#CC1(O)CCC2C3CCc4cc(O[Si](C)(C)C(C)(C)C)ccc4C3CCC21C  
**Mol. weight [g/mol]:** 410.66

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.62		Crippen Method
logp	6.291		Crippen Method
rinpol	3024.70		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U352390&Units=SI>  
**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)

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/43-646-7/17-alpha-Ethinylestradiol-3-tert-butyl dimethylsilyl-ether.pdf>

Generated by Cheméo on 2024-04-20 12:00:37.853518997 +0000 UTC m=+15903686.774096308.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.