

# «alpha»-Estradiol, bis(tert-butyldimethylsilyl) ether

<b>Other names:</b>	(17«alpha»)-3,17-Bispyrrol[tert-butyl(dimethyl)silyl]oxymorphoestra-1,3,5(10)-triene 17«alpha»-Estradiol, TBDMS 17«ALPHA»-estradiol, 2tbdms derivative
<b>Inchi:</b>	InChI=1S/C30H52O2Si2/c1-28(2,3)33(8,9)31-22-13-15-23-21(20-22)12-14-25-24(23)18-
<b>InchiKey:</b>	JFLALYDXWVIVJI-UHFFFAOYSA-N
<b>Formula:</b>	C30H52O2Si2
<b>SMILES:</b>	CC12CCC3c4ccc(O[Si](C)(C)C(C)(C)C)cc4CCC3C1CCC2O[Si](C)(C)C(C)(C)C
<b>Mol. weight [g/mol]:</b>	500.90

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.37		Crippen Method
logp	9.317		Crippen Method
rinpol	3530.40		NIST Webbook
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## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U332919&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U332919&amp;Units=SI</a>

## Legend

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

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