

# 16-Oxoestradiol, TMS

<b>Inchi:</b>	InChI=1S/C24H36O3Si2/c1-24-13-12-19-18-11-9-17(26-28(2,3)4)14-16(18)8-10-20(19)2
<b>InchiKey:</b>	LFFOMNXPQKCPPR-JDQHOHPRSA-N
<b>Formula:</b>	C24H36O3Si2
<b>SMILES:</b>	CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1C=C(O[Si](C)(C)C)C2=O
<b>Mol. weight [g/mol]:</b>	428.71

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	6.281		Crippen Method
rinpol	2689.00		NIST Webbook
rinpol	2712.00		NIST Webbook
rinpol	2689.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R525634&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R525634&amp;Units=SI</a>
<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>

## 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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<https://www.chemeo.com/cid/45-168-6/16-Oxoestradiol-TMS.pdf>

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