

# Methoxyoestrone (enol)-TMS

<b>Other names:</b>	4-Methoxyoestrone, TMS
<b>Inchi:</b>	InChI=1S/C25H40O3Si2/c1-25-16-15-18-17-11-13-22(27-29(3,4)5)24(26-2)20(17)10-9-1
<b>InchiKey:</b>	OUBUBDDLNRBPBN-AAANETGISA-N
<b>Formula:</b>	C25H40O3Si2
<b>SMILES:</b>	COc1c(O[Si](C)(C)C)ccc2c1CCC1C2CCC2(C)C(O[Si](C)(C)C)=CCC12
<b>Mol. weight [g/mol]:</b>	444.75

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Crippen Method
logp	7.110		Crippen Method
rinpola	2687.00		NIST Webbook
rinpola	2634.00		NIST Webbook
rinpola	2687.00		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=R166408&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R166408&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>rinpola:</b>	Non-polar retention indices

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<https://www.chemeo.com/cid/21-191-6/Methoxyoestrone-enol-TMS.pdf>

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