

# 6-Dehydroestrone (enol), TMS

**Inchi:** InChI=1S/C24H36O2Si2/c1-24-15-14-20-19-11-9-18(25-27(2,3)4)16-17(19)8-10-21(20)2  
**InchiKey:** NJFWRYVQKSEMQH-XRCKSUEFSA-N  
**Formula:** C24H36O2Si2  
**SMILES:** CC12CCC3c4ccc(O[Si](C)(C)C)cc4C=CC3C1CC=C2O[Si](C)(C)C  
**Mol. weight [g/mol]:** 412.71

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	7.182		Crippen Method
rinpol	2642.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R166428&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

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<https://www.chemeo.com/cid/15-704-3/6-Dehydroestrone-enol-TMS.pdf>

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