

# Estradiol, VDMS

**Inchi:** InChI=1S/C26H40O2Si2/c1-8-29(4,5)27-20-11-13-21-19(18-20)10-12-23-22(21)16-17-26  
**InchiKey:** UMKNFDWBBYRMIO-FZPKUJNRSA-N  
**Formula:** C26H40O2Si2  
**SMILES:** C=C[Si](C)(C)Oc1ccc2c(c1)CCC1C2CCC2(C)C(O[Si](C)(C)C=C)CCC12  
**Mol. weight [g/mol]:** 440.77

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.58		Crippen Method
logp	7.167		Crippen Method
rinpol	2856.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529567&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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/54-696-0/Estradiol-VDMS.pdf>

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