

# Silane, [(17«beta»)-2-methoxyestra-1,3,5(10)-triene-3,17-

Other names:

2-Methoxyoestradiol, bis-TMS

2-Methoxy-3,17-bis[(trimethylsilyl)oxy]estra-1,3,5(10)-triene, (17«beta»)-

2-Methoxyoestradiol, TMS

(17«beta»)-2-Methoxy-3,17-bis[(trimethylsilyl)oxy]estra-1(10),2,4-triene

2-Methoxyestradiol, 2tms derivative

**Inchi:** InChI=1S/C25H42O3Si2/c1-25-14-13-18-19(21(25)11-12-24(25)28-30(6,7)8)10-9-17-15-

**InchiKey:** FLTQSMBAZOOLHF-UIMGTSHQSA-N

**Formula:** C25H42O3Si2

**SMILES:** COc1cc2c(cc1O[Si](C)(C)C)CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12

**Mol. weight [g/mol]:** 446.77

**CAS:** 29825-47-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	6.985		Crippen Method
rinpol	2769.00		NIST Webbook
rinpol	2782.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C29825476&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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