# 11-Ketoestradiol (enol), TMS

**Inchi:** InChI=1S/C27H46O3Si3/c1-27-18-24(29-32(5,6)7)26-21-14-12-20(28-31(2,3)4)17-19(21)
**InchiKey:** PPBFFDCVRWUUNH-ORLBZUTRSA-N
**Formula:** C27H46O3Si3
**SMILES:** CC12C=C(O[Si](C)(C)C)C3c4ccc(O[Si](C)(C)C)cc4CCC3C1CCC2O[Si](C)(C)C
**Mol. weight [g/mol]:** 502.91

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -1.61 | | Crippen Method |
| logp | 7.932 | | Crippen Method |
| rinpol | 2903.00 | | NIST Webbook |
| rinpol | 2906.00 | | NIST Webbook |
| rinpol | 2903.00 | | NIST Webbook |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R166304&Units=SI

## Legend

**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**rinpol:** Non-polar retention indices