# 22-Ketocholesterol, TMS

**Inchi:** InChI=1S/C30H54O2Si/c1-20(2)9-14-28(31)21(3)25-12-13-26-24-11-10-22-19-23(32-33(
**InchiKey:** IAPAOYQMECJWJT-DARJXMCLSA-N
**Formula:** C30H54O2Si
**SMILES:** CC(C)CCC(=O)C(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
**Mol. weight [g/mol]:** 474.83

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -6.31 | | Crippen Method |
| logp | 8.507 | | Crippen Method |
| rinpol | 3290.00 | | 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=R528688&Units=SI

## Legend

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