

# 6,7-dehydro-11-keto-methylprednisolone, diMO-diTMS (1)

**Inchi:** InChI=1S/C30H48N2O5Si2/c1-20-16-22-23-13-15-30(37-39(9,10)11,26(32-35-5)19-36-3  
**InchiKey:** DGTIXRGNNMOEFD-BGLVPXFKSA-N  
**Formula:** C30H48N2O5Si2  
**SMILES:** CON=C1CC2(C)C(CCC2(O[Si](C)(C)C)C(CO[Si](C)(C)C)=NOC)C2C=C(C)C3=CC(=O)C  
**Mol. weight [g/mol]:** 572.88

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.46   |      | Crippen Method |
| logp          | 6.517   |      | Crippen Method |
| rinpol        | 3195.00 |      | NIST Webbook   |
| rinpol        | 3195.00 |      | NIST Webbook   |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R252049&Units=SI>

## Legend

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

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