

# ent-6«alpha»,7«alpha»-(OH)2 KA, MeTMS

**Inchi:** InChI=1S/C27H48O4Si2/c1-18-16-27-17-19(18)12-13-20(27)25(2)14-11-15-26(3,24(28)29)/h1-10,12-14,16-17,20-21,23-24,26-27,29-30,32-33H,11H2,31H3/t1,13,15,19,25,27,29,31,33/s1,13,15,19,25,27,29,31,33  
**InchiKey:** CKTNFGJOVXLXMW-CMXDAODCSA-N  
**Formula:** C27H48O4Si2  
**SMILES:** C=C1CC23CC1CCC2C1(C)CCCC(C)(C(=O)OC)C1C(O[Si](C)(C)C)C3O[Si](C)(C)C  
**Mol. weight [g/mol]:** 492.84

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| logp          | 6.788   |      | Crippen Method |
| rinpol        | 2582.00 |      | NIST Webbook   |
| rinpol        | 2581.00 |      | NIST Webbook   |
| rinpol        | 2588.00 |      | NIST Webbook   |
| rinpol        | 2582.00 |      | NIST Webbook   |
| rinpol        | 2593.00 |      | NIST Webbook   |
| rinpol        | 2581.00 |      | NIST Webbook   |
| rinpol        | 2593.00 |      | NIST Webbook   |

## Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R299355&Units=SI>

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)

Cheméo Relay (1.0):

## Legend

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/121-416-5/ent-6-alpha-7-alpha-OH-2-KA-MeTMS.pdf>

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