

# cis-Isohumulone, TMS

**Inchi:** InChI=1S/C29H54O4Si3/c1-21(2)16-17-24-27(30)26(25(20-23(5)6)31-34(7,8)9)28(32-35)29(36-39)4-3  
**InchiKey:** XFHXXWFFWSCATK-DJSDQNLUSA-N  
**Formula:** C<sub>29</sub>H<sub>54</sub>O<sub>4</sub>Si<sub>3</sub>  
**SMILES:** CC(C)=CCC1C(=O)C(C(=CC(C)C)O[Si](C)(C)C)=C(O[Si](C)(C)C)C1(CC=C(C)C)O[Si](C)(C)C  
**Mol. weight [g/mol]:** 550.99

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.58   |      | Crippen Method |
| logp          | 8.985   |      | Crippen Method |
| rinpol        | 2614.00 |      | NIST Webbook   |
| rinpol        | 2614.00 |      | 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=R96977&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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<https://www.chemeo.com/cid/29-930-7/cis-Isohumulone-TMS.pdf>

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