

# trans-Isoadhumulone, TMS

**Inchi:** InChI=1S/C27H46O5Si2/c1-13-20(6)24(29)23-25(30)21(16-14-18(2)3)27(32-34(10,11)12  
**InchiKey:** QHGGPAUBGUQBCS-PNSJCDHTSA-N  
**Formula:** C27H46O5Si2  
**SMILES:** CCC(C)C(=O)C1=C(O[Si](C)(C)C)C(O[Si](C)(C)C)(C(=O)CC=C(C)C)C(CC=C(C)C)C1=C  
**Mol. weight [g/mol]:** 506.82

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Crippen Method
logp	6.778		Crippen Method
rinsol	2607.00		NIST Webbook
rinsol	2569.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R97125&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

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

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