

# cis-Humulonic acid, TMS

**Inchi:** InChI=1S/C24H46O4Si3/c1-17(2)14-15-19-22(26-29(5,6)7)21(20(25)16-18(3)4)24(28-31)  
**InchiKey:** GKDNWXXKZQPZPB-UHFFFAOYSA-N  
**Formula:** C24H46O4Si3  
**SMILES:** CC(C)=CCC1=C(O[Si](C)(C)C)C(C(=O)CC(C)C)=C(O[Si](C)(C)C)C1O[Si](C)(C)C  
**Mol. weight [g/mol]:** 482.88

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.88		Crippen Method
logp	7.403		Crippen Method
rinpol	2208.00		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2216.00		NIST Webbook
rinpol	2242.00		NIST Webbook
rinpol	2182.00		NIST Webbook
rinpol	2191.00		NIST Webbook
rinpol	2182.00		NIST Webbook
rinpol	2208.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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=R96945&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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