

# Ursolic acid 2TMS

**Inchi:** InChI=1S/C36H64O3Si2/c1-24-16-21-36(31(37)39-41(11,12)13)23-22-34(6)26(30(36)25)  
**InchiKey:** XKHSFOSRVMEQJH-UHFFFAOYSA-N  
**Formula:** C36H64O3Si2  
**SMILES:** CC1CCC2(C(=O)O[Si](C)(C)C)CCC3(C)C(=CCC4C5(C)CCC(O[Si](C)(C)C)C(C)(C)C5C  
**Mol. weight [g/mol]:** 601.06  
**CAS:** 1206693-38-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.97		Crippen Method
logp	10.242		Crippen Method
rinpola	3657.20		NIST Webbook
rinpola	3657.20		NIST Webbook

## Sources

**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=C1206693380&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

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

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