

# Shikimic acid (4TMS)

**Inchi:** InChI=1S/C19H42O5Si4/c1-25(2,3)21-16-13-15(19(20)24-28(10,11)12)14-17(22-26(4,5))  
**InchiKey:** LMFAUEGOCMAFIW-UHFFFAOYSA-N  
**Formula:** C<sub>19</sub>H<sub>42</sub>O<sub>5</sub>Si<sub>4</sub>  
**SMILES:** C[Si](C)(C)OC(=O)C1=CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1  
**Mol. weight [g/mol]:** 462.88

## Physical Properties

Property code	Value	Unit	Source
log10ws	3.81		Crippen Method
logp	5.355		Crippen Method
rinpol	1794.80		NIST Webbook
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## 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=U413967&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/119-831-7/Shikimic-acid-4TMS.pdf>

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