

# Caffeic acid, ethyl ester, 2TMS

**Inchi:** InChI=1S/C17H28O4Si2/c1-8-19-17(18)12-10-14-9-11-15(20-22(2,3)4)16(13-14)21-23(5)  
**InchiKey:** GLKHKASGUMUKIA-ZRDIBKRKSA-N  
**Formula:** C17H28O4Si2  
**SMILES:** CCOC(=O)C=Cc1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1  
**Mol. weight [g/mol]:** 352.57

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.43		Crippen Method
logp	4.690		Crippen Method
rinpol	2081.40		NIST Webbook
rinpol	2081.40		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=U414032&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/122-682-9/Caffeic-acid-ethyl-ester-2TMS.pdf>

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