

# Caffeoylquinic acid, TMS

**Inchi:** InChI=1S/C34H66O9Si6/c1-44(2,3)38-27-21-19-26(23-28(27)39-45(4,5)6)20-22-31(35)3  
**InchiKey:** ZUMPKHAQJVFOSF-XDUBOXGASA-N  
**Formula:** C34H66O9Si6  
**SMILES:** C[Si](C)(C)OC(=O)C1(O[Si](C)(C)C)CC(OC(=O)C=Cc2ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)  
**Mol. weight [g/mol]:** 787.40

## Physical Properties

Property code	Value	Unit	Source
log10ws	3.78		Crippen Method
logp	9.241		Crippen Method
rinpol	3116.00		NIST Webbook
rinpol	3116.00		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=R631348&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/71-614-1/Caffeoylquinic-acid-TMS.pdf>

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