

# 4-O-Coumaroyl-D-quinic acid, 5TMS

**Inchi:** InChI=1S/C31H58O8Si5/c1-40(2,3)35-25-19-16-24(17-20-25)18-21-28(32)34-29-26(36-4  
**InchiKey:** LYICCCGATPPUNL-DYTRJAOYSA-N  
**Formula:** C31H58O8Si5  
**SMILES:** C[Si](C)(C)OC(=O)C1(O[Si](C)(C)C)CC(O[Si](C)(C)C)C(OC(=O)C=Cc2ccc(O[Si](C)(C)C)C  
**Mol. weight [g/mol]:** 699.21  
**CAS:** 179231-13-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	2.79		Crippen Method
logp	8.028		Crippen Method
rinpol	3025.90		NIST Webbook
rinpol	3025.90		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C179231131&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

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

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