# 3-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)34-26-22-31(3
**InchiKey:** NJXINYMXFRUJJM-DYTRJAOYSA-N
**Formula:** C31H58O8Si5
**SMILES:** C[Si](C)(C)OC(=O)C1(O[Si](C)(C)C)CC(OC(=O)C=Cc2ccc(O[Si](C)(C)C)cc2)C(O[Si](C)(
**Mol. weight [g/mol]:** 699.21
**CAS:** 179465-94-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | 2.79 | | Crippen Method |
| logp | 8.028 | | Crippen Method |
| rinpol | 3048.00 | | NIST Webbook |
| rinpol | 2962.10 | | NIST Webbook |
| rinpol | 2962.10 | | NIST Webbook |
| rinpol | 3048.00 | | NIST Webbook |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C179231120&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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