

# Quininic acid (5TMS)

**Inchi:** InChI=1S/C22H52O6Si5/c1-29(2,3)24-18-16-22(28-33(13,14)15,21(23)27-32(10,11)12)1  
**InchiKey:** DBCLHKSGLLGXOV-UHFFFAOYSA-N  
**Formula:** C22H52O6Si5  
**SMILES:** C[Si](C)(C)OC(=O)C1(O[Si](C)(C)C)CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1  
**Mol. weight [g/mol]:** 553.07

## Physical Properties

Property code	Value	Unit	Source
log10ws	5.16		Crippen Method
logp	6.409		Crippen Method
rinpol	1839.60		NIST Webbook
rinpol	1863.00		NIST Webbook
rinpol	1863.00		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=U413965&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/70-934-7/Quininic-acid-5TMS.pdf>

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