

# Citraconic acid, MO TBDMS # 2

**Inchi:** InChI=1S/C17H34O4Si2/c1-13(15(19)21-23(10,11)17(5,6)7)12-14(18)20-22(8,9)16(2,3)4  
**InchiKey:** HUKRUXTVYKXRNV-SEYXRHQNSA-N  
**Formula:** C17H34O4Si2  
**SMILES:** CC(=CC(=O)O[Si](C)(C)C(C)(C)C(=O)O[Si](C)(C)C(C)(C)C  
**Mol. weight [g/mol]:** 358.62

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.62		Crippen Method
logp	5.029		Crippen Method
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R564095&Units=SI>  
**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)

## 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/121-215-8/Citraconic-acid-MO-TBDMS-2.pdf>

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