

# Itaconic acid, bis(tert-butyldimethylsilyl) ester

**Other names:** Itaconic acid, TBDMS  
Itaconic acid, DMTBS  
Itaconic acid, 2tdms derivative

**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:** YPXRTKMWVGKUQN-UHFFFAOYSA-N

**Formula:** C17H34O4Si2

**SMILES:** C=C(CC(=O)O[Si](C)(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	1781.10		NIST Webbook
rinpol	1788.00		NIST Webbook
rinpol	1788.79		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1781.10		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=U352594&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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