

# 2-Pentenedioic acid, 3-methyl-, bis(trimethylsilyl) ester

Other names:

3-Methylglutaconic acid, bis(trimethylsilyl) ester

3-Methylglutaconic acid, di(trimethylsilyl) ester

3-Methylglutaconic acid, di-TMS

Bis(trimethylsilyl) 3-methyl-2-pentenedioate

3-Methylglutaconic acid, di-TMS ester

3-Methylglutaconic acid, di-TMS, #2

3-Methylglutaconic acid, di-TMS, #1

**Inchi:** InChI=1S/C12H24O4Si2/c1-10(8-11(13)15-17(2,3)4)9-12(14)16-18(5,6)7/h8H,9H2,1-7H3

**InchiKey:** CWJVRLKZONLMHK-CSKARUKUSA-N

**Formula:** C12H24O4Si2

**SMILES:** CC(=CC(=O)O[Si](C)(C)C)CC(=O)O[Si](C)(C)C

**Mol. weight [g/mol]:** 288.49

**CAS:** 55887-63-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	1.47		Crippen Method
logp	3.079		Crippen Method
rinpol	1441.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1491.00		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=C55887633&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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