

# Heptanedioic acid, bis(trimethylsilyl) ester

**Other names:**

Pimelic acid, bis(trimethylsilyl)-, ester  
Pimelic acid (2TMS)  
Heptanedioic acid, bis-TMS ester  
Pimelic acid, bis-TMS  
Pimelic acid, diTMS  
Heptanedioic acid, 1,7-bis(trimethylsilyl) ester  
Pimelic acid (tms)  
Heptanedioic acid, TMS ester  
Pimelic acid, 2tms derivative

**Inchi:**

InChI=1S/C13H28O4Si2/c1-18(2,3)16-12(14)10-8-7-9-11-13(15)17-19(4,5)6/h7-11H2,1-6

**InchiKey:**

VOLKRTUGJXKFMI-UHFFFAOYSA-N

**Formula:**

C<sub>13</sub>H<sub>28</sub>O<sub>4</sub>Si<sub>2</sub>

**SMILES:**

C[Si](C)(C)OC(=O)CCCCCC(=O)O[Si](C)(C)C

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

304.53

**CAS:**

55530-58-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.91		Crippen Method
logp	3.693		Crippen Method
rinpol	1591.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1592.00		NIST Webbook

# Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55530580&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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