

# Heptanedioic acid, bis(tert-butyldimethylsilyl) ester

<b>Other names:</b>	Pimelic acid, bis(tert-butyldimethylsilyl) ester Pimelic acid, diTBDMS Pimelic acid, DMTBS Pimelic acid, TBDMS Bis[tert-butyl(dimethyl)silyl] pimelate Heptanedioic acid, 2tbdms derivative
<b>Inchi:</b>	InChI=1S/C19H40O4Si2/c1-18(2,3)24(7,8)22-16(20)14-12-11-13-15-17(21)23-25(9,10)19
<b>InchiKey:</b>	BBMNMSUSTQGVGW-UHFFFAOYSA-N
<b>Formula:</b>	C19H40O4Si2
<b>SMILES:</b>	CC(C)(C)[Si](C)(C)OC(=O)CCCCC(=O)O[Si](C)(C)C(C)(C)C
<b>Mol. weight [g/mol]:</b>	388.69
<b>CAS:</b>	104255-95-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.60		Crippen Method
logp	6.034		Crippen Method
rinpol	2071.00		NIST Webbook
rinpol	2066.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2071.00		NIST Webbook
rinpol	2066.00		NIST Webbook
rinpol	2059.80		NIST Webbook
rinpol	2059.80		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C104255950&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C104255950&amp;Units=SI</a>

# Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**rinpol:** Non-polar retention indices

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