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/ci990307l
Crippen Method:	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