Butanedioic acid, methylene-, bis(trimethylsilyl) ester

Other names:	Itaconic acid (2TMS)
	Itaconic acid, di-TMS
	Itaconic acid, bis-TMS ester
	Mesaconic acid, di-TMS
	Itaconic acid (tms)
	Mesaconic acid, TMS
	Itaconic acid, 2tms derivative
Inchi:	InChI=1S/C11H22O4Si2/c1-9(11(13)15-17(5,6)7)8-10(12)14-16(2,3)4/h1,8H2,2-7H3
InchiKey:	IYEWOPPVIQNFQO-UHFFFAOYSA-N
Formula:	C11H22O4Si2
SMILES:	C=C(CC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	274.46
CAS:	55494-04-7

Physical Properties

Property code	Value	Unit	Source
log10ws	1.89		Crippen Method
logp	2.689		Crippen Method
rinpol	1400.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1419.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55494047&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Latest version available from:

https://www.chemeo.com/cid/38-952-3/Butanedioic-acid-methylene-bis-trimethylsilyl-ester.pdf

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