Bis(dimethyl-t-butylsilyl) fumarate

Other names:	2-Butenedioic acid, bis-DMTBS
	Fumaric acid, diTBDMS
	Fumaric acid, bis-TBDMS ester
	Fumaric acid, TBDMS
	Fumaric acid, DMTBS
	2-Butenedioic acid, (e)-, 2tbdms derivative
Inchi:	InChI=1S/C16H32O4Si2/c1-15(2,3)21(7,8)19-13(17)11-12-14(18)20-22(9,10)16(4,5)6/h1
InchiKey:	DDBSDNFXXPFNND-VAWYXSNFSA-N
Formula:	C16H32O4Si2
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)C=CC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	344.59
CAS:	99461-81-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.20		Crippen Method
logp	4.639		Crippen Method
rinpol	1786.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1787.00		NIST Webbook
rinpol	1786.39		NIST Webbook
rinpol	1787.00		NIST Webbook
rinpol	1779.00		NIST Webbook
rinpol	1786.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99461811&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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