2-Butenedioic acid (e)-, bis(trimethylsilyl) ester

Other names:	Fumaric acid, bis(trimethylsilyl) ester
	Bis(trimethylsilyl) fumarate
	Fumaric acid, bis-TMS ester
	Bis(trimethylsilyl) (2E)-2-butenedioate
	Fumaric acid (2TMS)
	Fumaric acid, bis-TMS
	Fumaric acid, di-TMS
	Fumaric acid (tms)
	2-Butenedioic acid, (e)-, 2tms derivative
Inchi:	InChI=1S/C10H20O4Si2/c1-15(2,3)13-9(11)7-8-10(12)14-16(4,5)6/h7-8H,1-6H3/b8-7+
InchiKey:	OITVFMRNHJZOHF-BQYQJAHWSA-N
Formula:	C10H20O4Si2
SMILES:	C[Si](C)(C)OC(=O)/C=C/C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	260.44

Physical Properties

Property code	Value	Unit	Source
ie	10.36	eV	Cheméo Relay (1.0)
log10ws	-2.86		Cheméo Relay (1.0)
logp	2.299		Crippen Method
rinpol	1349.00		NIST Webbook
rinpol	1345.50		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1349.00		NIST Webbook

rinpol	1353.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1360.00		NIST Webbook
tb	497.96	K	Cheméo Relay (1.0)
tf	332.17	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17962037&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point