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=CC(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 260.43

CAS: 17962-03-7

Physical Properties

Property code	Value	Unit	Source
log10ws	2.31		Crippen Method
logp	2.299		Crippen Method
rinpol	1349.00		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	1326.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1345.50		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

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17962037&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