2-Butenoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names: Trimethylsilyl 2-[(trimethylsilyl)oxy]-2-butenoate
2-Ketobutyric acid, enol, di-TMS
2-Ketobutyric acid, enol, bis-TMS
2-Ketobutyric acid, enol, di-TMS, #1
2-Ketobutyric acid, enol, di-TMS, #2
2-Ketobutyric acid, TMS

Inchi: InChI=1S/C10H22O3Si2/c1-8-9(12-14(2,3)4)10(11)13-15(5,6)7/h8H,1-7H3/b9-8-

InchiKey: ANZIASHOQWFLTL-HJWRWDBZSA-N

Formula: C10H22O3Si2

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

Mol. weight [g/mol]: 246.45

CAS: 55590-70-0

Physical Properties

Property code	Value	Unit	Source
log10ws	1.59		Crippen Method
logp	3.120		Crippen Method
rinpol	1186.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1186.00		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=C55590700&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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