

2-Butenoic acid, 2-methyl-, trimethylsilyl ester, (E)-

Other names:	Trimethylsilyl (2E)-2-methyl-2-butenoate Tiglic acid, mono-TMS Tiglic acid, TMS trans-2,3-Dimethylacrylic acid, trimethylsilyl ester Tiglic acid, tms derivative
Inchi:	InChI=1S/C8H16O2Si/c1-6-7(2)8(9)10-11(3,4)5/h6H,1-5H3/b7-6-
InchiKey:	GZQWHCAXPCOMTD-SREVYHEPSA-N
Formula:	C8H16O2Si
SMILES:	CC=C(C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	172.30
CAS:	55517-33-4

Physical Properties

Property code	Value	Unit	Source
log10ws	0.06		Crippen Method
logp	2.331		Crippen Method
rinpol	1014.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1008.20		NIST Webbook
rinpol	1014.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55517334&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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