

2-Butenoic acid, 3-methyl-2-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:	Trimethylsilyl 3-methyl-2-[(trimethylsilyl)oxy]-2-butenate 2-Ketovaleric acid, enol, di-TMS 2-Ketoisocaproic acid, enol, di-TMS
Inchi:	InChI=1S/C11H24O3Si2/c1-9(2)10(13-15(3,4)5)11(12)14-16(6,7)8/h1-8H3
InchiKey:	MSIWTYHCYLOUFV-UHFFFAOYSA-N
Formula:	C11H24O3Si2
SMILES:	CC(C)=C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	260.48
CAS:	55044-79-6

Physical Properties

Property code	Value	Unit	Source
log10ws	1.17		Crippen Method
logp	3.510		Crippen Method
rinpola	1261.00		NIST Webbook
rinpola	1261.00		NIST Webbook
rinpola	1282.00		NIST Webbook
rinpola	1262.00		NIST Webbook
rinpola	1262.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55044796&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
rinpola:	Non-polar retention indices

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