

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

Other names:

2-Keto-3-methylvaleric acid, enol, di-TMS

2-Keto-3-methylvaleric acid, enol, (2TMS)

2-Keto-3-methylvaleric acid, enol, TMS

Inchi:

InChI=1S/C12H26O3Si2/c1-9-10(2)11(14-16(3,4)5)12(13)15-17(6,7)8/h9H2,1-8H3/b11-1

InchiKey:

RHJGXCQRZWTGMA-KHPPLWFESA-N

Formula:

C<sub>12</sub>H<sub>26</sub>O<sub>3</sub>Si<sub>2</sub>

SMILES:

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

Mol. weight [g/mol]:

274.50

CAS:

55320-09-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.75		Crippen Method
logp	3.900		Crippen Method
rmpol	1325.00		NIST Webbook
rmpol	1318.00		NIST Webbook
rmpol	1327.00		NIST Webbook
rmpol	1314.00		NIST Webbook
rmpol	1314.00		NIST Webbook

## Sources

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C55320097&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

rmpol:

Non-polar retention indices

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