

2-Methyl-3-ketobutyric acid, enol, TMS

Other names:	2-Methyl-3-ketobutyric acid, enol, di-TMS
Inchi:	InChI=1S/C11H24O3Si2/c1-9(10(2)13-15(3,4)5)11(12)14-16(6,7)8/h1-8H3/b10-9-
InchiKey:	BDEWTIHUFJXUDU-KTKRTIGZSA-N
Formula:	C11H24O3Si2
SMILES:	CC(O[Si](C)(C)C)=C(C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	260.48

Physical Properties

Property code	Value	Unit	Source
log10ws	1.17		Crippen Method
logp	3.510		Crippen Method
rinpola	1328.00		NIST Webbook
rinpola	1278.00		NIST Webbook
rinpola	1327.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R51389&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/70-414-4/2-Methyl-3-ketobutyric-acid-enol-TMS.pdf>

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