

2-Methylacetoacetic acid, di(trimethylsilyl) deriv.

Other names:	Trimethylsilyl 2-methyl-3-[(trimethylsilyl)oxy]-2-butenate 2-Methylacetoacetic acid, bis-TMS Acetoacetic acid, 2-methyl, (2TMS)- Acetoacetic acid, 2-methyl, 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-MDZDMXLPSA-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
CAS:	98779-02-3

Physical Properties

Property code	Value	Unit	Source
log10ws	1.17		Crippen Method
logp	3.510		Crippen Method
rinpol	1320.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1320.00		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=C98779023&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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