

# Acetoacetic acid, bis(trimethylsilyl)- deriv.

<b>Other names:</b>	Acetoacetic acid, di(trimethylsilyl) deriv. Acetoacetic acid, bis(trimethylsilyl)- Trimethylsilyl 3-[(trimethylsilyl)oxy]-2-butenate 3-Ketobutyric acid, enol, di-TMS Acetoacetic acid, bis-TMS Acetoacetic acid, diTMS Acetoacetic acid, (2TMS) Acetoacetic acid, TMS 3-Ketobutyric acid, enol, di-TMS, #2 3-Ketobutyric acid, enol, di-TMS, #1
<b>Inchi:</b>	InChI=1S/C10H22O3Si2/c1-9(12-14(2,3)4)8-10(11)13-15(5,6)7/h8H,1-7H3/b9-8-
<b>InchiKey:</b>	VIWVQG UWKULKOS-HJWRWDBZSA-N
<b>Formula:</b>	C10H22O3Si2
<b>SMILES:</b>	CC(=CC(=O)O[Si](C)(C)C)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	246.45
<b>CAS:</b>	82326-10-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	1.59		Crippen Method
logp	3.120		Crippen Method
rinqol	1243.00		NIST Webbook
rinqol	1207.00		NIST Webbook
rinqol	1254.00		NIST Webbook
rinqol	1213.00		NIST Webbook
rinqol	1255.00		NIST Webbook
rinqol	1204.00		NIST Webbook
rinqol	1249.00		NIST Webbook
rinqol	1200.00		NIST Webbook
rinqol	1240.00		NIST Webbook
rinqol	1204.00		NIST Webbook
rinqol	1243.00		NIST Webbook
rinqol	1221.00		NIST Webbook
rinqol	1249.00		NIST Webbook
rinqol	1204.00		NIST Webbook
rinqol	1221.00		NIST Webbook

# Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C82326101&Units=SI>

# Legend

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

Latest version available from:

<https://www.chemeo.com/cid/29-687-8/Acetoacetic-acid-bis-trimethylsilyl-deriv.pdf>

Generated by Cheméo on 2024-04-26 20:40:43.532631331 +0000 UTC m=+16453292.453208728.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.