Acetoacetic acid, bis(trimethylsilyl)- deriv.

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

Physical Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	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