

Oximated acetoacetic acid, diTMS

Other names:	Acetoacetic acid, oxime, bis-TMS
Inchi:	InChI=1S/C10H23NO3Si2/c1-9(11-14-16(5,6)7)8-10(12)13-15(2,3)4/h8H2,1-7H3/b11-9+
InchiKey:	TZPNNUWYLUYPBF-PKNNBQFBNSA-N
Formula:	C10H23NO3Si2
SMILES:	CC(CC(=O)O[Si](C)(C)C)=NO[Si](C)(C)C
Mol. weight [g/mol]:	261.47

Physical Properties

Property code	Value	Unit	Source
log10ws	1.79		Crippen Method
logp	2.982		Crippen Method
rinpol	1261.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1252.00		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=R112931&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/124-069-8/Oximated-acetoacetic-acid-diTMS.pdf>

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