

3-Ketobutyric acid, oxime, di-TMS, #2

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-PKNCBQFBNSA-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	1275.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1275.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R51599&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.cheméo.com/cid/122-047-4/3-Ketobutyric-acid-oxime-di-TMS-2.pdf>

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