

2-Ketovaleric acid ho-tms

Other names:	2-Ketopentanoic acid ho-tms 2-Ketovaleric acid, oxime, di-TMS 2-Oxopentanoic acid, oxime, bis-TMS 2-Ketovaleric acid, oxime, TMS
Inchi:	InChI=1S/C11H25NO3Si2/c1-8-9-10(12-15-17(5,6)7)11(13)14-16(2,3)4/h8-9H2,1-7H3
InchiKey:	LTRLDUKRPZFIGZ-UHFFFAOYSA-N
Formula:	C11H25NO3Si2
SMILES:	CCCC(=NO[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	275.49

Physical Properties

Property code	Value	Unit	Source
log10ws	1.37		Crippen Method
logp	3.372		Crippen Method
rinpol	1265.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1263.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332273&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/11-463-5/2-Ketovaleric-acid-ho-tms.pdf>

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