

# 3-Methyl-2-ketobutyric acid pfbo-tms

<b>Other names:</b>	Isovaleric acid, 2-oxo, O-pentafluorobenzyloxime, TMS
<b>Inchi:</b>	InChI=1S/C15H18F5NO3Si/c1-7(2)14(15(22)24-25(3,4)5)21-23-6-8-9(16)11(18)13(20)12
<b>InchiKey:</b>	CEGBIHR CNHPYPQ-UHFFFAOYSA-N
<b>Formula:</b>	C15H18F5NO3Si
<b>SMILES:</b>	CC(C)C(=NOCc1c(F)c(F)c(F)c(F)c1F)C(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	383.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	4.289		Crippen Method
rinpola	1537.00		NIST Webbook
rinpola	1556.00		NIST Webbook
rinpola	1537.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U332300&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U332300&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>rinpola:</b>	Non-polar retention indices

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