

# Acetoacetic acid, O-pentafluorobenzoyloxime, TMS

Inchi:	InChI=1S/C14H16F5NO3Si/c1-7(5-9(21)23-24(2,3)4)20-22-6-8-10(15)12(17)14(19)13(18)
InchiKey:	BTULZGHAJIMZPV-IFRROFPPSA-N
Formula:	C14H16F5NO3Si
SMILES:	CC(CC(=O)O[Si](C)(C)C)=NOc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	369.36

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	4.043		Crippen Method
rinpol	1570.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1570.00		NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R315383&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R315383&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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