

3-Trimethylsilyloxy-2-methylpyran-4-one

Other names:	3-Hydroxy-2-methyl-pyran-4-one TMS
Inchi:	InChI=1S/C9H14O3Si/c1-7-9(12-13(2,3)4)8(10)5-6-11-7/h5-6H,1-4H3
InchiKey:	JAMVNVJEEYSRKJ-UHFFFAOYSA-N
Formula:	C9H14O3Si
SMILES:	<chem>Cc1occc(=O)c1O[Si](C)(C)C</chem>
Mol. weight [g/mol]:	198.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	2.162		Crippen Method
rinpol	1293.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373047&Units=SI

Legend

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

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<https://www.chemeo.com/cid/39-335-7/3-Trimethylsilyloxy-2-methylpyran-4-one.pdf>

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