

3-Hydroxy-2-butanone, trimethylsilyl ether

Other names:	3-[(Trimethylsilyl)oxy]butan-2-one Acetoin, tms derivative
Inchi:	InChI=1S/C7H16O2Si/c1-6(8)7(2)9-10(3,4)5/h7H,1-5H3
InchiKey:	SCHPFYABZNRJOB-UHFFFAOYSA-N
Formula:	C7H16O2Si
SMILES:	CC(=O)C(C)O[Si](C)(C)C
Mol. weight [g/mol]:	160.29

Physical Properties

Property code	Value	Unit	Source
log10ws	0.72		Crippen Method
logp	1.815		Crippen Method
rinpol	879.60		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333797&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.chemeo.com/cid/42-799-9/3-Hydroxy-2-butanone-trimethylsilyl-ether.pdf>

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