

3-Oxopentanoic acid, TMS

Other names:	3-Ketovaleric acid, TMS
Inchi:	InChI=1S/C8H16O3Si/c1-5-7(9)6-8(10)11-12(2,3)4/h5-6H2,1-4H3
InchiKey:	BOPHYICVYUYPGN-UHFFFAOYSA-N
Formula:	C8H16O3Si
SMILES:	CCC(=O)CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	188.30

Physical Properties

Property code	Value	Unit	Source
log10ws	0.64		Crippen Method
logp	1.734		Crippen Method
rinpola	1286.00		NIST Webbook
rinpola	1272.00		NIST Webbook
rinpola	1286.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R112897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/16-857-3/3-Oxopentanoic-acid-TMS.pdf>

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