

3-Methylvaleric acid, TMS

Inchi:	InChI=1S/C9H20O2Si/c1-6-8(2)7-9(10)11-12(3,4)5/h8H,6-7H2,1-5H3
InchiKey:	HYPLBXPWARHOLR-UHFFFAOYSA-N
Formula:	C9H20O2Si
SMILES:	CCC(C)CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	188.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.26		Crippen Method
logp	2.801		Crippen Method
rinpol	1059.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414250&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/98-882-5/3-Methylvaleric-acid-TMS.pdf>

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