

Butanoic acid, 3-methyl-, tert-butyldimethylsilyl ester

Other names:	Butanoic acid, 3-methyl, TBDMS Isovaleric acid, TBDMS Isovaleric acid, DMTBS 3-Methylbutanoic acid, tbdms derivative
Inchi:	InChI=1S/C11H24O2Si/c1-9(2)8-10(12)13-14(6,7)11(3,4)5/h9H,8H2,1-7H3
InchiKey:	OWWNBWBPVKVZEOB-UHFFFAOYSA-N
Formula:	C11H24O2Si
SMILES:	CC(C)CC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	216.39
CAS:	111864-22-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.10		Crippen Method
logp	3.581		Crippen Method
rinpol	1147.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111864223&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
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/98-675-5/Butanoic-acid-3-methyl-tert-butyldimethylsilyl-ester.pdf>

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