

3-Methyl-4-trimethylsiloxy(trimethylsilyl)butyrate

Other names:	Butanoic acid, 4-hydroxy-3-methyl, bis-TMS Butanoic acid, 3-methyl-4-trimethylsilyloxy, trimethylsilyl ester
Inchi:	InChI=1S/C11H26O3Si2/c1-10(9-13-15(2,3)4)8-11(12)14-16(5,6)7/h10H,8-9H2,1-7H3
InchiKey:	KIVDVHUDXOLIMU-UHFFFAOYSA-N
Formula:	C11H26O3Si2
SMILES:	CC(CO[Si](C)(C)C)CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	262.49

Physical Properties

Property code	Value	Unit	Source
log10ws	1.76		Crippen Method
logp	3.242		Crippen Method
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U78916&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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