

Propanoic acid, 2-methyl-, trimethylsilyl ester

Other names:	Isobutyric acid, trimethylsilyl ester Trimethylsilyl isobutyrate 2-Methylpropanoic acid, tms derivative
Inchi:	InChI=1S/C7H16O2Si/c1-6(2)7(8)9-10(3,4)5/h6H,1-5H3
InchiKey:	IHTVTNNAFDOJBO-UHFFFAOYSA-N
Formula:	C7H16O2Si
SMILES:	CC(C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	160.29
CAS:	16883-61-7

Physical Properties

Property code	Value	Unit	Source
log10ws	0.58		Crippen Method
logp	2.020		Crippen Method
rinpol	832.00		NIST Webbook
rinpol	832.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16883617&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/45-787-9/Propanoic-acid-2-methyl-trimethylsilyl-ester.pdf>

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