

Propanoic acid, 2-methyl-, tert-butyldimethylsilyl ester

Other names:	Propanoic acid, 2-methyl, TBDMS Isobutyric acid, DMTBS Isobutyric acid, TBDMS 2-Methylpropanoic acid, tbdms derivative
Inchi:	InChI=1S/C10H22O2Si/c1-8(2)9(11)12-13(6,7)10(3,4)5/h8H,1-7H3
InchiKey:	UPXVKHCBIBVPTJ-UHFFFAOYSA-N
Formula:	C10H22O2Si
SMILES:	CC(C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	202.37
CAS:	111864-21-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.68		Crippen Method
logp	3.191		Crippen Method
rinpol	1050.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1057.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111864212&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

Latest version available from:

<https://www.chemeo.com/cid/17-553-9/Propanoic-acid-2-methyl-tert-butyl-dimethylsilyl-ester.pdf>

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