

Butanoic acid, 2-oxo-, trimethylsilyl ester

Other names:	«alpha»-Ketobutyric acid, TMS 2-Ketobutyric acid, trimethylsilyl ester 2-Ketobutyric acid, tms derivative
Inchi:	InChI=1S/C7H14O3Si/c1-5-6(8)7(9)10-11(2,3)4/h5H2,1-4H3
InchiKey:	FDGFSLJBVKGLCO-UHFFFAOYSA-N
Formula:	C7H14O3Si
SMILES:	CCC(=O)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	174.27
CAS:	74367-68-3

Physical Properties

Property code	Value	Unit	Source
log10ws	1.05		Crippen Method
logp	1.344		Crippen Method
rinpol	989.80		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74367683&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/44-032-7/Butanoic-acid-2-oxo-trimethylsilyl-ester.pdf>

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