

Pentanoic acid, 2-oxo-, trimethylsilyl ester

Other names:	«alpha»-Ketovaleric acid, TMS 2-Ketovaleric acid, TMS ester 2-Ketovaleric acid, TMS # 1 2-Oxopentanoic acid, tms derivative
Inchi:	InChI=1S/C8H16O3Si/c1-5-6-7(9)8(10)11-12(2,3)4/h5-6H2,1-4H3
InchiKey:	KXURKMKWKFOXLN-UHFFFAOYSA-N
Formula:	C8H16O3Si
SMILES:	CCCC(=O)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	188.30
CAS:	74367-69-4

Physical Properties

Property code	Value	Unit	Source
log10ws	0.64		Crippen Method
logp	1.734		Crippen Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74367694&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

Latest version available from:

<https://www.chemeo.com/cid/24-657-6/Pentanoic-acid-2-oxo-trimethylsilyl-ester.pdf>

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