

Pentanoic acid, 4-oxo-, trimethylsilyl ester

Other names:	Laevulic acid, trimethylsilyl ester Laevulinic acid TMS
Inchi:	InChI=1S/C8H16O3Si/c1-7(9)5-6-8(10)11-12(2,3)4/h5-6H2,1-4H3
InchiKey:	SKSOOBJAPLSIMV-UHFFFAOYSA-N
Formula:	C8H16O3Si
SMILES:	CC(=O)CCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	188.30
CAS:	55557-12-5

Physical Properties

Property code	Value	Unit	Source
log10ws	0.64		Crippen Method
logp	1.734		Crippen Method
rinpol	1119.00		NIST Webbook
rinpol	1130.10		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55557125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/98-781-7/Pentanoic-acid-4-oxo-trimethylsilyl-ester.pdf>

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