

Pentenoic acid, 4-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:	Levulinic acid enol di-TMS Levulinic acid, TMS
Inchi:	InChI=1S/C11H24O3Si2/c1-10(13-15(2,3)4)8-9-11(12)14-16(5,6)7/h8H,9H2,1-7H3/b10-8
InchiKey:	QZDHQSBCOALOEZ-NTMALXAHS-A-N
Formula:	C11H24O3Si2
SMILES:	CC(=CCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	260.48
CAS:	72101-11-2

Physical Properties

Property code	Value	Unit	Source
log10ws	1.17		Crippen Method
logp	3.510		Crippen Method
rinpol	1279.00		NIST Webbook
rinpol	1279.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72101112&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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.cheméo.com/cid/114-877-2/Pentenoic-acid-4-trimethylsilyl-oxy-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-05-03 14:53:55.547751078 +0000 UTC m=+17037284.468328394.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.