

2-Pentenoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:	2-Ketoisovaleric acid, bis(trimethylsilyl)- 2-Methyl-3-ketobutyric acid, bis(trimethylsilyl)- 2-Ketovaleric acid, TMS # 3
Inchi:	InChI=1S/C11H24O3Si2/c1-8-9-10(13-15(2,3)4)11(12)14-16(5,6)7/h9H,8H2,1-7H3/b10-9
InchiKey:	OHSILHRTQNZRQH-KTKRTIGZSA-N
Formula:	C11H24O3Si2
SMILES:	CCC=C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	260.48
CAS:	55045-17-5

Physical Properties

Property code	Value	Unit	Source
log10ws	1.17		Crippen Method
logp	3.510		Crippen Method
rinpol	1314.00		NIST Webbook
rinpol	1314.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55045175&Units=SI

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/124-202-9/2-Pentenoic-acid-2-trimethylsilyl-oxy-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-30 09:29:34.255417293 +0000 UTC m=+16758623.175994607.
Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.