

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

Other names:	2-Ketocaproic acid, TMS # 2
Inchi:	InChI=1S/C12H26O3Si2/c1-8-9-10-11(14-16(2,3)4)12(13)15-17(5,6)7/h10H,8-9H2,1-7H3
InchiKey:	JZFKPHTPKLNAMQ-KHPPLWFESA-N
Formula:	C12H26O3Si2
SMILES:	CCCC=C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	274.50
CAS:	69796-61-8

Physical Properties

Property code	Value	Unit	Source
log10ws	0.75		Crippen Method
logp	3.900		Crippen Method
rinpola	1338.00		NIST Webbook
rinpola	1338.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69796618&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpola:	Non-polar retention indices

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<https://www.chemeo.com/cid/120-404-9/2-Hexenoic-acid-2-trimethylsilyl-oxy-trimethylsilyl-ester.pdf>

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