

# Hexanoic acid, 3-trimethylsilyloxy, trimethylsilyl ester

Other names:

Trimethylsilyl 3-[(trimethylsilyl)oxy]hexanoate

3-Trimethylsilyloxy(trimethylsilyl)caproate

3-Trimethylsilyloxy(trimethylsilyl)caproate

3-Hydroxycaproic acid, bis-TMS

Caproic acid, 3-hydroxy, di-TMS

3-Hydroxycaproic acid, TMS

Inchi:

InChI=1S/C12H28O3Si2/c1-8-9-11(14-16(2,3)4)10-12(13)15-17(5,6)7/h11H,8-10H2,1-7H

InchiKey:

TUSDZUHTPDSVRW-UHFFFAOYSA-N

Formula:

C<sub>12</sub>H<sub>28</sub>O<sub>3</sub>Si<sub>2</sub>

SMILES:

CCCC(CC(=O)O[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]:

276.52

CAS:

136788-82-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.99		Crippen Method
logp	3.775		Crippen Method
rinpol	1317.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1317.00		NIST Webbook

## Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C136788824&Units=SI>

## Legend

log10ws:

Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices

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