

3-TRIMETHYLSILOXY(TRIMETHYLSILYL)CAPROATE

Other names:	3-Hydroxycaproic acid, TMS
	3-Hydroxycaproic acid, bis-TMS
	3-Trimethylsiloxy(trimethylsilyl)caproate
	3-Trimethylsilyloxy(trimethylsilyl)caproate
	Caproic acid, 3-hydroxy, di-TMS
	Trimethylsilyl 3-[(trimethylsilyl)oxy]hexanoate
Inchi:	InChI=1S/C12H28O3Si2/c1-8-9-11(14-16(2,3)4)10-12(13)15-17(5,6)7/h11H,8-10H2,1-7H3
InchiKey:	TUSDZUHTPDSVRW-UHFFFAOYSA-N
Formula:	C12H28O3Si2
SMILES:	CCCC(CC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	276.52

Physical Properties

Property code	Value	Unit	Source
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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

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

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/20-318-6/3-TRIMETHYLSILOXY-TRIMETHYLSILYL-CAPROATE.pdf>

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