

Bis(trimethyl) derivative of 5-Hydroxyhexanoic acid

Other names:

5-Hydroxyhexanoic acid diTMS

5-Hydroxycaproic acid, di-TMS

Hexanoic acid, 5-trimethylsilyloxy, trimethylsilyl ester

Inchi:

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

InchiKey:

ZBACSLBZHSAYHX-UHFFFAOYSA-N

Formula:

C₁₂H₂₈O₃Si₂

SMILES:

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

Mol. weight [g/mol]:

276.52

CAS:

79628-63-0

Physical Properties

Property code	Value	Unit	Source
log10ws	0.99		Crippen Method
logp	3.775		Crippen Method
rinpol	1370.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1370.00		NIST Webbook

Sources

Crippen Method:

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

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C79628630&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.cheméo.com/cid/55-317-9/Bis-trimethyl-derivative-of-5-Hydroxyhexanoic-acid.pdf>

Generated by Cheméo on 2024-04-28 21:08:04.163446405 +0000 UTC m=+16627733.084023717.

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