

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

Other names:

2-Hydroxyhexanoic acid di-TMS
2-Hydroxycaproic acid, bis-TMS
2-Hydroxycaproic acid, trimethylsilyl ether, trimethylsilyl ester
2-Hydroxycaproic acid, TMS

Inchi:

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

InchiKey:

RQWYRMABBIFEGY-UHFFFAOYSA-N

Formula:

C12H28O3Si2

SMILES:

CCCCC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]:

276.52

CAS:

54890-07-2

Physical Properties

Property code	Value	Unit	Source
log10ws	0.99		Crippen Method
logp	3.775		Crippen Method
rinpol	1284.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1289.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C54890072&Units=SI>

Crippen Method:

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

Crippen Method:

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

Legend

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

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