

Pentanoic acid, 4-methyl-2-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:

2-Hydroxyisocaproic acid, di-TMS

2-Hydroxyisocaproic acid, bis-TMS

Pentanoic acid, 2-hydroxy-4-methyl, (2TMS)-

2-Hydroxyisocaproic acid, TMS

Pentanoic acid, 2-hydroxy-4-methyl, TMS

2-Hydroxyisocaproic acid, 2tms derivative

Inchi: InChI=1S/C12H28O3Si2/c1-10(2)9-11(14-16(3,4)5)12(13)15-17(6,7)8/h10-11H,9H2,1-8H

InchiKey: BTVVIFVNNGJOJY-UHFFFAOYSA-N

Formula: C12H28O3Si2

SMILES: CC(C)CC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 276.52

CAS: 54890-08-3

Physical Properties

Property code	Value	Unit	Source
log10ws	1.23		Crippen Method
logp	3.631		Crippen Method
rinpol	1238.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1226.90		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1242.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C54890083&Units=SI>

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

Legend

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

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