

Pentanoic acid, 3-methyl-2-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:

2-Hydroxy-3-methylvaleric acid, di-TMS

2-Hydroxy-3-methylvaleric acid, (2TMS)-

2-Hydroxy-3-methylvaleric acid, TMS

Inchi:

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

InchiKey:

DJXWAEIPSSKZGI-UHFFFAOYSA-N

Formula:

C₁₂H₂₈O₃Si₂

SMILES:

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

Mol. weight [g/mol]:

276.52

CAS:

54890-09-4

Physical Properties

Property code	Value	Unit	Source
log10ws	1.23		Crippen Method
logp	3.631		Crippen Method
rinpol	1250.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1253.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C54890094&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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