

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

Other names:
ester

3-Trimethylsilyloxyisovaleric acid, trimethylsilyl ester

«beta»-Hydroxyisovaleric acid, trimethylsilyl ether, trimethylsilyl ester

3-Hydroxyisovaleric acid, bis-TMS

3-Hydroxyisovaleric acid, di-TMS

Butanoic acid, 3-methyl, 3-hydroxy, (2TMS)-

Butanoic acid, 3-methyl, 3-hydroxy, TMS

3-Hydroxyisovaleric acid, 2tms derivative

Inchi: InChI=1S/C11H26O3Si2/c1-11(2,14-16(6,7)8)9-10(12)13-15(3,4)5/h9H2,1-8H3

InchiKey: CEMBCVWMQGTNRL-UHFFFAOYSA-N

Formula: C11H26O3Si2

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

Mol. weight [g/mol]: 262.49

CAS: 55124-90-8

Physical Properties

Property code	Value	Unit	Source
log10ws	1.41		Crippen Method
logp	3.385		Crippen Method
rinpol	1216.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1217.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1203.90		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1203.90		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C55124908&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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