

Butanoic acid, 3-methyl-2-[(trimethylsilyloxy)-, trimethylsilyl

Other names:
ester

«alpha»-Hydroxyisovaleric acid, (2TMS)-

2-Hydroxyisopentanoic acid, bis-TMS

2-Hydroxyisovaleric acid, di-TMS

Butanoic acid, 2-hydroxy-3-methyl, bis-TMS

Isovaleric acid, 2-hydroxy, di-TMS

2-Hydroxyisovaleric acid, TMS

2-Hydroxyisovalerate, TMS

2-Hydroxy-3-methylbutyric acid, 2tms derivative

Inchi: InChI=1S/C11H26O3Si2/c1-9(2)10(13-15(3,4)5)11(12)14-16(6,7)8/h9-10H,1-8H3

InchiKey: QWRWSWPAGNHCNI-UHFFFAOYSA-N

Formula: C11H26O3Si2

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

Mol. weight [g/mol]: 262.49

CAS: 55124-92-0

Physical Properties

Property code	Value	Unit	Source
log10ws	1.65		Crippen Method
logp	3.241		Crippen Method
rinpol	1174.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1175.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55124920&Units=SI>

Legend

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

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