

Butanoic acid, 2-[(tert-butyl(dimethylsilyl)oxy]-3-methyl-, tert-butyl(dimethylsilyl) ester

Other names:

2-Hydroxyisovaleric acid, bis-TBDMS
2-Hydroxyisovaleric acid, diTBDMS
2-Hydroxyisovaleric acid, TBDMS ether, TBDMS ester
Butanoic acid, 2-hydroxy-3-methyl, bis-TBDMS
2-Hydroxyisovaleric acid, TBDMS
Butanoic acid, 2-hydroxy-3-methyl, TBDMS
2-Hydroxyisovaleric acid, DMTBS
2-Hydroxyisovalerate, TBDMS
2-Hydroxy-3-methylbutyric acid, 2tbdms derivative

Inchi: InChI=1S/C17H38O3Si2/c1-13(2)14(19-21(9,10)16(3,4)5)15(18)20-22(11,12)17(6,7)8/h1

InchiKey: NUIUNGHKCAVDFV-UHFFFAOYSA-N

Formula: C17H38O3Si2

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

Mol. weight [g/mol]: 346.65

CAS: 180784-67-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.86		Crippen Method
logp	5.581		Crippen Method
rinpol	1608.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1604.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C180784672&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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