

«beta»-Hydroxyisovaleric acid, O-(tert-butyl dimethylsilyl)-, tert-butyl dimethylsilyl ester

Other names: tert-Butyl(dimethyl)silyl 3-(tert-butyl dimethylsilyloxy)isobutyrate morpho-3-methylbutanoate 3-Hydroxyisovaleric acid, diTBDMS

3-Hydroxyisovaleric acid, 2tbdms derivative

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

InchiKey: PZSKMQJCHSQOOF-UHFFFAOYSA-N

Formula: C17H38O3Si2

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

Mol. weight [g/mol]: 346.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.10		Crippen Method
logp	5.725		Crippen Method
rinpol	1654.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1638.10		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1638.10		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=U333128&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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