

«alpha»-Hydroxyisobutyric acid, tert-butyl dimethylsilyl ether, tert-butyl dimethylsilyl ester

Other names: Propanoic acid, 2-hydroxy-2-methyl-, bis-DMTBS

Inchi: InChI=1S/C16H36O3Si2/c1-14(2,3)20(9,10)18-13(17)16(7,8)19-21(11,12)15(4,5)6/h1-12

InchiKey: SAAYCFHJLUOGNJ-UHFFFAOYSA-N

Formula: C16H36O3Si2

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

Mol. weight [g/mol]: 332.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.68		Crippen Method
logp	5.335		Crippen Method
rinpol	1498.90		NIST Webbook
rinpol	1498.90		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U221723&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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