

2-Methyl-3-hydroxybutyric acid, diTBDMS

Inchi: InChI=1S/C17H38O3Si2/c1-13(14(2)19-21(9,10)16(3,4)5)15(18)20-22(11,12)17(6,7)8/h1
InchiKey: WRYYXJJXANUFSZ-UHFFFAOYSA-N
Formula: C17H38O3Si2
SMILES: CC(O[Si](C)(C)C(C)(C)C(C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 346.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.86		Crippen Method
logp	5.581		Crippen Method
rinpol	1641.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R276570&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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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<https://www.cheméo.com/cid/55-937-1/2-Methyl-3-hydroxybutyric-acid-diTBDMS.pdf>

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