

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

Other names: (+/-)-3-Hydroxybutyric acid, tert-butyl dimethylsilyl ether, tert-butyl dimethylsilyl 3-Hydroxybutyric acid, diTBDMS

3-Hydroxybutyric acid, 2tdms derivative

Inchi: InChI=1S/C16H36O3Si2/c1-13(18-20(8,9)15(2,3)4)12-14(17)19-21(10,11)16(5,6)7/h13H

InchiKey: MTLHHAQBPSTUCQ-UHFFFAOYSA-N

Formula: C16H36O3Si2

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

Mol. weight [g/mol]: 332.63

CAS: 91998-39-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.68		Crippen Method
logp	5.335		Crippen Method
rinpol	1594.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1576.80		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=C91998399&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/39-968-5/Butanoic-acid-3-tert-butyldimethylsilyl-oxy-tert-butyldimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-23 06:01:54.339267302 +0000 UTC m=+16141363.259844617.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.