

Butanoic acid, 4-[(tert-butyl(dimethylsilyl)oxy]-, tert-butyl(dimethylsilyl) ester

Other names:

4-Hydroxybutyric acid, bi-TBDMS
Butanoic acid, 4-hydroxy, bis-TBDMS

4-Hydroxybutyric acid, bis-TBDMS

Butanoic acid, 4-hydroxy, TBDMS

4-Hydroxybutanoic acid, 2tdms derivative

Inchi:

InChI=1S/C16H36O3Si2/c1-15(2,3)20(7,8)18-13-11-12-14(17)19-21(9,10)16(4,5)6/h11-1

InchiKey:

HPXRSTXXSLXSCU-UHFFFAOYSA-N

Formula:

C16H36O3Si2

SMILES:

CC(C)(C)[Si](C)(C)OCCCC(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]:

332.63

CAS:

149357-72-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.57		Crippen Method
logp	5.337		Crippen Method
rinpol	1674.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1674.00		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=C149357722&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/36-233-3/Butanoic-acid-4-tert-butyl-dimethylsilyl-oxy-tert-butyl-dimethylsilyl-ester.pdf>

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