

(.+/-)-3-Hydroxybutyric acid, trimethylsilyl ether, trimethylsilyl ester

Other names: (.+/-)-3-Hydroxybutyric acid, 2tms derivative
Inchi: InChI=1S/C10H24O3Si2/c1-9(12-14(2,3)4)8-10(11)13-15(5,6)7/h9H,8H2,1-7H3
InchiKey: YWRIHOYCAHATJN-UHFFFAOYSA-N
Formula: C10H24O3Si2
SMILES: CC(CC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 248.47

Physical Properties

Property code	Value	Unit	Source
log10ws	1.83		Crippen Method
logp	2.995		Crippen Method
rinpol	1153.30		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=U333754&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.chemeo.com/cid/70-689-0/3-Hydroxybutyric-acid-trimethylsilyl-ether-trimethylsilyl-ester.pdf>

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