

3-Hydroxybutyric acid, mono-TBDMS # 1

Inchi: InChI=1S/C10H22O3Si/c1-8(11)7-9(12)13-14(5,6)10(2,3)4/h8,11H,7H2,1-6H3
InchiKey: FJQQDEOGLNWWEI-UHFFFAOYSA-N
Formula: C10H22O3Si
SMILES: CC(O)CC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 218.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.30		Crippen Method
logp	2.306		Crippen Method
rinpol	1241.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R563418&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/16-056-2/3-Hydroxybutyric-acid-mono-TBDMS-1.pdf>

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