Butanoic acid, 2,2-dimethyl-3-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names: 2,2-Dimethyl-3-trimethylsiloxy(trimethylsilyl)butyrate
2,2-Dimethyl-3-hydroxybutanoic acid, di-TMS

Inchi: InChI=1S/C12H28O3Si2/c1-10(14-16(4,5)6)12(2,3)11(13)15-17(7,8)9/h10H,1-9H3

InchiKey: DJCIAUQXAPLLSG-UHFFFAOYSA-N

Formula: C12H28O3Si2

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

Mol. weight [g/mol]: 276.52

CAS: 55530-56-8

Physical Properties

Property code	Value	Unit	Source
log10ws	1.23		Crippen Method
logp	3.631		Crippen Method
rinpol	1395.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1395.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55530568&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices