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

Other names:	(+/-)-3Hydroxybutyric acid, tert-butyldimethylsilyl ether, tert-butyldimethylsilyl ester 3-Hydroxybutyric acid, diTBDMS 3-Hydroxybutyric acid, 2tbdms 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/ci990307l
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