Pentanoic acid, 2-[(tert-butyldimethylsilyl)oxy]-4-methyl-, tert-butyldimethylsilyl ester

Other names:	2-Hydroxyisocaproic acid, diTBDMS
	2-Hydroxyisocaproic acid, bis-TBDMS
	2-Hydroxyisocaproic acid, TBDMS
	2-Hydroxyisocaproic acid, tert-butyldimethylsilyl ether, tert-butyldimethylsilyl ester
	2-Hydroxyisocaproic acid, DMTBS
	2-Hydroxyisocaproic acid, (s)-, 2tbdms derivative
Inchi:	InChI=1S/C18H40O3Si2/c1-14(2)13-15(20-22(9,10)17(3,4)5)16(19)21-23(11,12)18(6,7)8
InchiKey:	MUXPVGBUUPXKBR-UHFFFAOYSA-N
Formula:	C18H40O3Si2
SMILES:	CC(C)CC(O[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	360.68
CAS:	89682-23-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.28		Crippen Method
logp	5.971		Crippen Method
rinpol	1654.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1653.00		NIST Webbook
rinpol	1652.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89682235&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