

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(=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

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