L-Valine, N-(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Other names: N,O-Bis(dimethyl-t-butylsilyl)-l-valine
tert-Butyl(dimethyl)silyl 2-([tert-butyl(dimethyl)silyl]amino)-3-methylbutanoate, (L)-
Valine diTBDMS
Valine, bis-TBDMS
Val, bis-TBDMS
Val, TBDMS
Valine, TBDMS
L-valine, 2tbdms derivative

Inchi: InChI=1S/C17H39NO2Si2/c1-13(2)14(18-21(9,10)16(3,4)5)15(19)20-22(11,12)17(6,7)8/h

InchiKey: KPMGOLUDVQVDCW-UHFFFAOYSA-N

Formula: C17H39NO2Si2

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

Mol. weight [g/mol]: 345.67

CAS: 107715-89-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.96		Crippen Method
logp	5.154		Crippen Method
rinpol	1659.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1642.30		NIST Webbook
rinpol	1684.00		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=C107715899&Units=SI

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/68-391-3/L-Valine-N-tert-butyldimethylsilyl-tert-butyldimethylsilyl-ester.pdf
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