

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

Other names: tert-Butyl(dimethyl)silyl 2-((tert-butyl(dimethyl)silyl)amino)propanoate
Alanine diTBDMS
Ala, O,N-bis-DMTBS
Ala, TBDMS
tert-Butyl(dimethyl)silyl 2-((tert-butyl(dimethyl)silyl)amino)propanoate, (S)-
Ala, N,O-di-TBDMS
Alanine, N,O-bis-TBDMS
Alanine, TBDMS
L-alanine, 2tdms derivative

Inchi: InChI=1S/C15H35NO2Si2/c1-12(16-19(8,9)14(2,3)4)13(17)18-20(10,11)15(5,6)7/h12,16

InchiKey: NZMBBDALTGCDPQ-GFCCVEGCSA-N

Formula: C15H35NO2Si2

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

Mol. weight [g/mol]: 317.61

CAS: 92751-15-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.37		Crippen Method
logp	4.518		Crippen Method
rinpol	1540.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1524.30		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1524.30		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1540.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C92751150&Units=SI>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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