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

Other names: N,O-Bis(dimethyl-t-butylsilyl)-l-phenylalanine
tert-Butyl(dimethyl)silyl 2-([tert-butyl(dimethyl)silyl]amino)-3-phenylpropanoate, (L)-
Phenylalanine, diTBDMS
Phenylalanine, N,O-bis-TBDMS
Phe, N,O-bis-TBDMS
Phe, TBDMS
Phenylalanine, TBDMS
L-phenylalanine, 2tbdms derivative

Inchi: InChI=1S/C21H39NO2Si2/c1-20(2,3)25(7,8)22-18(16-17-14-12-11-13-15-17)19(23)24-26

InchiKey: CCHAQKAMPRPVGP-GOSISDBHSA-N

Formula: C21H39NO2Si2

SMILES: CC(C)(C)[Si](C)(C)NC(Cc1ccccc1)C(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 393.71

CAS: 107715-95-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.98		Crippen Method
logp	5.741		Crippen Method
rinpol	2098.00		NIST Webbook
rinpol	2091.20		NIST Webbook
rinpol	2094.00		NIST Webbook
rinpol	2094.00		NIST Webbook
rinpol	2091.20		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2098.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C107715957&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