

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: | CCHAQKAMPRPVG-P-GOSISDBHSA-N |
| Formula: | C ₂₁ H ₃₉ NO ₂ Si ₂ |
| SMILES: | <chem>CC(C)(C)[Si](C)(C)NC(Cc1ccccc1)C(=O)O[Si](C)(C)C(C)(C)C</chem> |
| 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/ci9903071 |

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.cheméo.com/cid/120-888-3/L-Phenylalanine-N-tert-butyldimethylsilyl-tert-butyldimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-29 11:20:54.784775339 +0000 UTC m=+16678903.705352654.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.