

# 4-Pyridoxic acid, bis(tert-butyl dimethylsilyl) ether, tert-butyl dimethylsilyl ester

**Other names:** 4-Pyridoxic acid, 3tdms derivative; Pyridoxic acid, TBDMS; tert-Butyl(dimethyl)silyl 3-pyrrol[tert-butyl(dimethyl)silyl]oxymorpho-5-(pyrrol[tert-butyl(dimethyl)silyl]oxymorphomethyl)-2-methylisonicotinate.

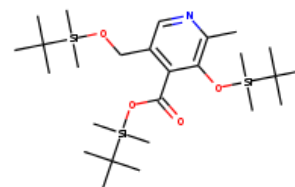
**InChI:** InChI=1S/C26H51NO4Si3/c1-19-22(30-33(13,14)25(5,6)7)21(23(28)31-34(15,16)26(8,9)10)20(17-27-19)18-29-32(11,12)24(2,3)4/h17H,18H2,1-16H3

**InChI Key:** QJCSWPQIEJTJMG-UHFFFAOYSA-N

**Formula:** C<sub>26</sub>H<sub>51</sub>NO<sub>4</sub>Si<sub>3</sub>

**SMILES:** Cc1ncc(CO[Si](C)(C)C(C)(C)C)c(C(=O)O[Si](C)(C)C(C)(C)C)c1O[Si](C)(C)C(C)(C)C

**Molecular Weight:** 525.94



## Physical Properties

| Property                  | Value | Unit | Source         |
|---------------------------|-------|------|----------------|
| $\log P_{\text{oct/wat}}$ | 8.46  |      | Crippen Method |

## Sources

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C26H51NO4Si3/c1-19-22\(30-33\(13,14\)25\(5,6\)7\)21\(23\(28\)31-34\(15,16\)26\(8,9\)10\)20\(17-27-19\)18-29-32\(11,12\)24\(2,3\)4/h17H,18H2,1-16H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C26H51NO4Si3/c1-19-22(30-33(13,14)25(5,6)7)21(23(28)31-34(15,16)26(8,9)10)20(17-27-19)18-29-32(11,12)24(2,3)4/h17H,18H2,1-16H3)

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

## Legend

$\log P_{\text{oct/wat}}$ : Octanol/Water partition coefficient .

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