

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

Other names: tert-Butyl(dimethyl)silyl
3-pyrro[tert-butyl(dimethyl)silyl]oxymorpho-5-(pyrro[tert-butyl(dimethyl)silyl]oxymorphom
Pyridoxic acid, TBDMS
4-Pyridoxic acid, 3tbdms derivative

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)

InchiKey: QJCSWPQIEJTJMG-UHFFFAOYSA-N

Formula: C26H51NO4Si3

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

Mol. weight [g/mol]: 525.94

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	8.458		Crippen Method
rinpol	2600.90		NIST Webbook
rinpol	2630.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333508&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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