4-Pyridoxic acid, bis(trimethylsilyl) ether, trimethylsilyl ester

Other names: Trimethylsilyl 2-methyl-3-[(trimethylsilyl)oxy]-5-pyrrol[(trimethylsilyl)oxy]methylmorphoisonicotinate
4-Pyridoxic acid, tris-TMS
Pyridoxic acid, TMS
4-Pyridoxic acid, TMS
Pyridoxic acid, 3tms derivative

Inchi: InChI=1S/C17H33NO4Si3/c1-13-16(21-24(5,6)7)15(17(19)22-25(8,9)10)14(11-18-13)12-

InchiKey: HSIPISKXEKPCKY-UHFFFAOYSA-N

Formula: C17H33NO4Si3

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

Mol. weight [g/mol]: 399.70

Physical Properties

Property code	Value	Unit	Source
log10ws	0.88		Crippen Method
logp	4.947		Crippen Method
rinpol	1966.00		NIST Webbook
rinpol	1934.70		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	1934.70		NIST Webbook
rinpol	1966.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333509&Units=SI

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices