Pyridoxamine, TMS

Inchi: InChI=1S/C17H36N2O2Si3/c1-14-17(21-24(8,9)10)16(12-19-22(2,3)4)15(11-18-14)13-20
InchiKey: LJLIAHFEXPDFCB-UHFFFAOYSA-N
Formula: C17H36N2O2Si3
SMILES: Cc1ncc(CO[Si](C)(C)C)c(CN[Si](C)(C)C)c1O[Si](C)(C)C
Mol. weight [g/mol]: 384.74

Physical Properties

Property code	Value	Unit	Source
log10ws	0.63		Crippen Method
logp	4.880		Crippen Method
rinpol	1948.00		NIST Webbook
rinpol	1972.00		NIST Webbook
rinpol	1972.00		NIST Webbook
rinpol	1948.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R95327&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