2-[[tert-Butyl(dimethyl)silyl](methyl)amino]-1-(4-py

Other names: 2-[[tert-Butyl(dimethyl)silyl](methyl)amino]-1-(4-{[tert-butyl(dimethyl)silyl]oxy}-3-methoxyph
Metanephrine, n-2tbdms derivative
Inchi: InChI=1S/C22H43NO3Si2/c1-21(2,3)27(9,10)23(7)16-18(24)17-13-14-19(20(15-17)25-8)
InchiKey: IDSRSXAUPMIXDC-UHFFFAOYSA-N
Formula: C22H43NO3Si2
SMILES: COc1cc(C(O)CN(C)[Si](C)(C)C(C)(C)C)ccc1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 425.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.93		Crippen Method
logp	6.050		Crippen Method
rinpol	2534.20		NIST Webbook
rinpol	2534.20		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U334025&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices