dl-Metanephrine, bis(tert-butyldimethylsilyl) ether

Other names: Metanephrine, 2tbdms derivative
Inchi: InChI=1S/C22H43NO3Si2/c1-21(2,3)27(9,10)25-18-14-13-17(15-19(18)24-8)20(16-23-7)
InchiKey: ZLTAOLBLYQYGNN-UHFFFAOYSA-N
Formula: C22H43NO3Si2
SMILES: CNCC(O[Si](C)(C)C(C)(C)C)c1ccc(O[Si](C)(C)C(C)(C)C)c(OC)c1
Mol. weight [g/mol]: 425.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	6.361		Crippen Method
rinpol	2239.80		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U334024&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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