dl-Metanephrine, N,O,O'-(tert-butyldimethylsilyl)-

Other names: Metanephrine, 3tbdms derivative
Inchi: InChI=1S/C28H57NO3Si3/c1-26(2,3)33(12,13)29(10)21-25(32-35(16,17)28(7,8)9)22-18-
InchiKey: RJQGCVMWZCITDE-UHFFFAOYSA-N
Formula: C28H57NO3Si3
SMILES: COc1cc(C(CN(C)[Si](C)(C)C(C)(C)C)O[Si](C)(C)C(C)(C)C)ccc1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 540.01

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.32		Crippen Method
logp	9.079		Crippen Method
rinpol	2592.00		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=U334026&Units=SI

Legend

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