

# Metanephrine, N-isoBOC, O-TBDMS

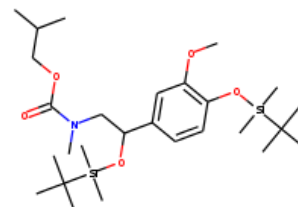
**InChI:** InChI=1S/C27H51NO5Si2/c1-20(2)19-31-25(29)28(9)18-24(33-35(13,14)27(6,7)8)21-15-16-22(23(17-21)30-10)32-34(11,12)26(3,4)5/h15-17,20,24H,18-19H2,1-14H3

**InChI Key:** AJXZZQAJAMFCDW-UHFFFAOYSA-N

**Formula:** C27H51NO5Si2

**SMILES:** COc1cc(C(CN(C)C(=O)OCC(C)C)O[Si](C)(C)C(C)C)ccc1O[Si](C)(C)C(C)C

**Molecular Weight:** 525.87



## Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	7.87		Crippen Method

## Sources

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C27H51NO5Si2/c1-20\(2\)19-31-25\(29\)28\(9\)18-24\(33-35\(13,14\)27\(6,7\)8\)21-15-16-22\(23\(17-21\)30-10\)32-34\(11,12\)26\(3,4\)5/h15-17,20,24H,18-19H2,1-14H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C27H51NO5Si2/c1-20(2)19-31-25(29)28(9)18-24(33-35(13,14)27(6,7)8)21-15-16-22(23(17-21)30-10)32-34(11,12)26(3,4)5/h15-17,20,24H,18-19H2,1-14H3)

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

$\log P_{\text{oct/wat}}$ : Octanol/Water partition coefficient .

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