

# 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-  
**InchiKey:** AJXZZQAJAMFCDW-UHFFFAOYSA-N  
**Formula:** C27H51NO5Si2  
**SMILES:** COc1cc(C(CN(C)C(=O)OCC(C)C)O[Si](C)(C)C(C)(C)C)ccc1O[Si](C)(C)C(C)(C)C  
**Mol. weight [g/mol]:** 525.87

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	7.866		Crippen Method
rinpol	2866.00		NIST Webbook
rinpol	2866.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R392746&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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

Latest version available from:

<https://www.chemeo.com/cid/49-343-7/Metanephrine-N-isoBOC-O-TBDMS.pdf>

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