# Methanimine, 1-(1-pyrrolidinyl), N-(3-methoxyphenyl)

**Inchi:** InChI=1S/C12H16N2O/c1-15-12-6-4-5-11(9-12)13-10-14-7-2-3-8-14/h4-6,9-10H,2-3,7-8H

**InchiKey:** YLRSDZWACKZGEG-UHFFFAOYSA-N

**Formula:** C12H16N2O

**SMILES:** COc1cccc(N=CN2CCCC2)c1

**Mol. weight [g/mol]:** 204.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -2.37 | | Crippen Method |
| logp | 2.451 | | Crippen Method |
| mcvol | 166.850 | ml/mol | McGowan Method |
| rinpol | 1985.00 | | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R118944&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices