

# Methanimine, 1-(1-pyrrolidiny), N-(4-bromophenyl)

**Inchi:** InChI=1S/C11H13BrN2/c12-10-3-5-11(6-4-10)13-9-14-7-1-2-8-14/h3-6,9H,1-2,7-8H2/b13  
**InchiKey:** ZDMVZMGCMZEGBJ-UKTHLTGXSA-N  
**Formula:** C11H13BrN2  
**SMILES:** BrC1ccc(N=CN2CCCC2)cc1  
**Mol. weight [g/mol]:** 253.14

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	3.205		Crippen Method
mcvol	164.390	ml/mol	McGowan Method
rinpole	2060.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R118979&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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  
**rinpole:** Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/13-980-9/Methanimine-1-1-pyrrolidiny-N-4-bromophenyl.pdf>

Generated by Cheméo on 2024-04-26 08:23:15.840697175 +0000 UTC m=+16409044.761274491.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.