

# Formamidine, 3,3-hexamethylene-1-(3-bromophenyl)

**Inchi:** InChI=1S/C13H17BrN2/c14-12-6-5-7-13(10-12)15-11-16-8-3-1-2-4-9-16/h5-7,10-11H,1-4  
**InchiKey:** OLFIGLWUCZBNEM-RVDMUPIBSA-N  
**Formula:** C13H17BrN2  
**SMILES:** BrC1CCCC(N=CN2CCCCCC2)c1  
**Mol. weight [g/mol]:** 281.19

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Crippen Method
logp	3.985		Crippen Method
mcvol	192.570	ml/mol	McGowan Method
rinpola	2217.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R118553&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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  
**mcvol:** McGowan's characteristic volume  
**rinpola:** Non-polar retention indices

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