

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

**Inchi:** InChI=1S/C13H17N3O2/c17-16(18)13-7-5-6-12(10-13)14-11-15-8-3-1-2-4-9-15/h5-7,10-12  
**InchiKey:** FCHCZTAAHITZRM-UHFFFAOYSA-N  
**Formula:** C13H17N3O2  
**SMILES:** O=[N+]([O-])c1cccc(N=CN2CCCCC2)c1  
**Mol. weight [g/mol]:** 247.29

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	3.131		Crippen Method
mcvol	192.490	ml/mol	McGowan Method
rinpol	2366.00		NIST Webbook
rinpol	2366.00		NIST Webbook

## Sources

**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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R118602&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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