

# 2,2'-Bipyrimidine

**Inchi:** InChI=1S/C8H6N4/c1-3-9-7(10-4-1)8-11-5-2-6-12-8/h1-6H  
**InchiKey:** HKOAFLAGUQUJQG-UHFFFAOYSA-N  
**Formula:** C8H6N4  
**SMILES:** c1cnc(-c2ncccn2)nc1  
**Mol. weight [g/mol]:** 158.16  
**CAS:** 34671-83-5

## Physical Properties

Property code	Value	Unit	Source
ie	8.30	eV	NIST Webbook
ie	9.17	eV	NIST Webbook
log10ws	-3.14		Crippen Method
logp	0.934		Crippen Method
mcvol	115.980	ml/mol	McGowan Method

## 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=C34671835&Units=SI>

## Legend

**ie:** Ionization energy  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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