

# 4-Nitropyridine

**Inchi:** InChI=1S/C5H4N2O2/c8-7(9)5-1-3-6-4-2-5/h1-4H  
**InchiKey:** FEXIEMAAKBNTFK-UHFFFAOYSA-N  
**Formula:** C5H4N2O2  
**SMILES:** O=[N+]([O-])c1ccncc1  
**Mol. weight [g/mol]:** 124.10  
**CAS:** 1122-61-8

## Physical Properties

Property code	Value	Unit	Source
affp	874.30	kJ/mol	NIST Webbook
basg	842.50	kJ/mol	NIST Webbook
ie	10.20 ± 0.10	eV	NIST Webbook
ie	10.40	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	0.990		Crippen Method
mcvol	84.950	ml/mol	McGowan Method

## Sources

**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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1122618&Units=SI&Mask=3FFF>

## Legend

**affp:** Proton affinity  
**basg:** Gas basicity  
**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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