

# 1-azabicyclo[2.2.2]-octane, 3-cyano

**Inchi:** InChI=1S/C8H12N2/c9-5-8-6-10-3-1-7(8)2-4-10/h7-8H,1-4,6H2  
**InchiKey:** ICSMHHPNBLZOLB-UHFFFAOYSA-N  
**Formula:** C8H12N2  
**SMILES:** N#CC1CN2CCCC1CC2  
**Mol. weight [g/mol]:** 136.19  
**CAS:** 51627-76-0

## Physical Properties

Property code	Value	Unit	Source
affp	935.40	kJ/mol	NIST Webbook
basg	904.60	kJ/mol	NIST Webbook
log10ws	-0.91		Crippen Method
logp	0.852		Crippen Method
mcvol	113.220	ml/mol	McGowan Method

## Sources

**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=C51627760&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**affp:** Proton affinity  
**basg:** Gas basicity  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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