

# 3-Amino-1-azabicyclo[2.2.2]octane

**Other names:** (+-)-3-Aminoquinuclidine  
**Inchi:** InChI=1S/C7H14N2/c8-7-5-9-3-1-6(7)2-4-9/h6-7H,1-5,8H2  
**InchiKey:** REUAXQZIRFXQML-UHFFFAOYSA-N  
**Formula:** C7H14N2  
**SMILES:** NC1CN2CCC1CC2  
**Mol. weight [g/mol]:** 126.20  
**CAS:** 6238-14-8

## Physical Properties

Property code	Value	Unit	Source
affp	985.50	kJ/mol	NIST Webbook
basg	954.70	kJ/mol	NIST Webbook
ie	7.96	eV	NIST Webbook
log10ws	-0.42		Crippen Method
logp	0.039		Crippen Method
mcvol	107.730	ml/mol	McGowan Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C6238148&Units=SI>  
**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>

## 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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