

# 2-Azabicyclo[2.2.2]octane-2-carboxylic acid, 5-oxo-, ethyl ester

**Other names:** 2-Ethoxycarbonyl-2-azabicyclo[2.2.2]octan-5-one  
**Inchi:** InChI=1S/C10H15NO3/c1-2-14-10(13)11-6-7-3-4-8(11)5-9(7)12/h7-8H,2-6H2,1H3  
**InchiKey:** GCHPMC MRBLSVMZ-UHFFFAOYSA-N  
**Formula:** C10H15NO3  
**SMILES:** CCOC(=O)N1CC2CCC1CC2=O  
**Mol. weight [g/mol]:** 197.23  
**CAS:** 37778-51-1

## Physical Properties

Property code	Value	Unit	Source
ie	8.50	eV	NIST Webbook
ie	8.89	eV	NIST Webbook
log10ws	-1.36		Crippen Method
logp	1.196		Crippen Method
mcvol	149.030	ml/mol	McGowan Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C37778511&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)

## 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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