

# 2-Azabicyclo[2.2.2]oct-5-ene-2-carboxylic acid, ethyl ester

Other names:	2-Ethoxycarbonyl-2-azabicyclo[2.2.2]oct-5-ene
Inchi:	InChI=1S/C10H15NO2/c1-2-13-10(12)11-7-8-3-5-9(11)6-4-8/h3,5,8-9H,2,4,6-7H2,1H3
InchiKey:	LZSYMBPNSZCLIC-UHFFFAOYSA-N
Formula:	C10H15NO2
SMILES:	CCOC(=O)N1CC2C=CC1CC2
Mol. weight [g/mol]:	181.23
CAS:	3693-69-4

## Physical Properties

Property code	Value	Unit	Source
ie	8.00	eV	NIST Webbook
ie	8.52	eV	NIST Webbook
log10ws	-1.93		Crippen Method
logp	1.793		Crippen Method
mcvol	143.160	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3693694&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3693694&amp;Units=SI</a>

## 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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