

# 1-Azabicyclo[2.2.2]octane, 4-ethyl-

<b>Inchi:</b>	InChI=1S/C9H17N/c1-2-9-3-6-10(7-4-9)8-5-9/h2-8H2,1H3
<b>InchiKey:</b>	ZLPCABMSTVWUGB-UHFFFAOYSA-N
<b>Formula:</b>	C9H17N
<b>SMILES:</b>	CCC12CCN(CC1)CC2
<b>Mol. weight [g/mol]:</b>	139.24
<b>CAS:</b>	45732-65-8

## Physical Properties

Property code	Value	Unit	Source
ie	8.05 ± 0.01	eV	NIST Webbook
log10ws	-1.71		Crippen Method
logp	1.882		Crippen Method
mcvol	125.930	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C45732658&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C45732658&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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