

# 5-Azabenzimidazole

<b>Other names:</b>	1H-Imidazo(4,5-c)pyridine 3,5-Diazaindole
<b>Inchi:</b>	InChI=1S/C6H5N3/c1-2-7-3-6-5(1)8-4-9-6/h1-4H,(H,8,9)
<b>InchiKey:</b>	UBOOKRVGOBKDMM-UHFFFAOYSA-N
<b>Formula:</b>	C6H5N3
<b>SMILES:</b>	<chem>c1cc2nc[nH]c2cn1</chem>
<b>Mol. weight [g/mol]:</b>	119.12
<b>CAS:</b>	272-97-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Crippen Method
logp	0.476		Crippen Method
mcvol	86.420	ml/mol	McGowan Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C272979&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C272979&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## Legend

<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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