

# Betazole

<b>Other names:</b>	1H-Pyrazole-3-ethanamine Pyrazole, 3-(2-aminoethyl)- Ametazole 3-(2-Aminoethyl)pyrazole 3-Aminoethylpyrazole
<b>Inchi:</b>	InChI=1S/C5H9N3/c6-3-1-5-2-4-7-8-5/h2,4H,1,3,6H2,(H,7,8)
<b>InchiKey:</b>	JXDFAQONERDKSS-UHFFFAOYSA-N
<b>Formula:</b>	C5H9N3
<b>SMILES:</b>	NCCc1cc[nH]n1
<b>Mol. weight [g/mol]:</b>	111.15
<b>CAS:</b>	105-20-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.69		Crippen Method
logp	-0.571		Crippen Method
mcvol	91.790	ml/mol	McGowan Method
rinpol	1390.00		NIST Webbook
rinpol	1390.00		NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.50 ± 2.50	K	0.07	NIST Webbook

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C105204&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C105204&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>

# 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
<b>rinpol:</b>	Non-polar retention indices
<b>tbrp:</b>	Boiling point at reduced pressure

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