

# N-(2-Cyanoethyl)-pyrrole

<b>Other names:</b>	1H-Pyrrole-1-propanenitrile Pyrrole-1-propionitrile 1-(2-Cyanoethyl)pyrrole 3-Pyrrolidinopropionitrile 3-(pyrrol-1-yl)propionitrile
<b>Inchi:</b>	InChI=1S/C7H8N2/c8-4-3-7-9-5-1-2-6-9/h1-2,5-6H,3,7H2
<b>InchiKey:</b>	IYOLJLGYJMJSU-UHFFFAOYSA-N
<b>Formula:</b>	C7H8N2
<b>SMILES:</b>	N#CCCN1CCCC1
<b>Mol. weight [g/mol]:</b>	120.15
<b>CAS:</b>	43036-06-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	1.402		Crippen Method
mcpvol	101.390	ml/mol	McGowan Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.70	K	1.30	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C43036062&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C43036062&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>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>tbrp:</b>	Boiling point at reduced pressure

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