

# 1-(2-Cyanoethyl)-2-ethyl-4-methylimidazole

<b>Other names:</b>	1H-Imidazole-1-propanenitrile, 2-ethyl-4-methyl-1-Cyanoethyl-2-ethyl-4-methylimidazole 2-ethyl-4-methyl-1H-imidazole-1-propionitrile
<b>Inchi:</b>	InChI=1S/C9H13N3/c1-3-9-11-8(2)7-12(9)6-4-5-10/h7H,3-4,6H2,1-2H3
<b>InchiKey:</b>	UIDDPPKZYZTEGS-UHFFFAOYSA-N
<b>Formula:</b>	C9H13N3
<b>SMILES:</b>	CCc1nc(C)cn1CCC#N
<b>Mol. weight [g/mol]:</b>	163.22
<b>CAS:</b>	23996-25-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	1.668		Crippen Method
mcvol	139.550	ml/mol	McGowan Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C23996250&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23996250&amp;Units=SI</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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