

# 2-Pyrazoline, 5-ethyl-3,5-dimethyl, N-acetyl

<b>Inchi:</b>	InChI=1S/C9H16N2O/c1-5-9(4)6-7(2)10-11(9)8(3)12/h5-6H2,1-4H3
<b>InchiKey:</b>	XJCKUHKNAUNIFP-UHFFFAOYSA-N
<b>Formula:</b>	C9H16N2O
<b>SMILES:</b>	CCC1(C)CC(C)=NN1C(C)=O
<b>Mol. weight [g/mol]:</b>	168.24

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.10		Crippen Method
logp	1.783		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
rinpole	1222.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R322980&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R322980&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>
<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>rinpole:</b>	Non-polar retention indices

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