

# 3-(5-methylfurfurylidene)-1-pyrroline, (E)

<b>Inchi:</b>	InChI=1S/C10H11NO/c1-8-2-3-10(12-8)6-9-4-5-11-7-9/h2-3,6-7H,4-5H2,1H3/b9-6+
<b>InchiKey:</b>	BCWSVRKZMCXABS-RMKNXTFCSA-N
<b>Formula:</b>	C10H11NO
<b>SMILES:</b>	Cc1ccc(C=C2C=NCC2)o1
<b>Mol. weight [g/mol]:</b>	161.20

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.82		Crippen Method
logp	2.446		Crippen Method
mcvol	128.690	ml/mol	McGowan Method
ripol	2135.00		NIST Webbook
ripol	2135.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R315338&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R315338&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>ripol:</b>	Polar retention indices

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