

# 1-Phenyl-3-acetoxy-2-pyrazoline

<b>Inchi:</b>	InChI=1S/C11H12N2O2/c1-9(14)15-11-7-8-13(12-11)10-5-3-2-4-6-10/h2-6H,7-8H2,1H3
<b>InchiKey:</b>	KEKBLIAQVPGFMT-UHFFFAOYSA-N
<b>Formula:</b>	C11H12N2O2
<b>SMILES:</b>	CC(=O)OC1=NN(c2ccccc2)CC1
<b>Mol. weight [g/mol]:</b>	204.23
<b>CAS:</b>	2748-21-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	1.773		Crippen Method
mcvol	154.330	ml/mol	McGowan Method

## Sources

<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=C2748212&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2748212&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>

## 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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