

# 1-Phenyl-2-acetyl-4-methyl-3-pyrazolidone

<b>Other names:</b>	2-acetyl-4-methyl-1-phenylpyrazolidin-3-one
<b>Inchi:</b>	InChI=1S/C12H14N2O2/c1-9-8-13(11-6-4-3-5-7-11)14(10(2)15)12(9)16/h3-7,9H,8H2,1-2
<b>InchiKey:</b>	BPNPRBBKUKZUCD-UHFFFAOYSA-N
<b>Formula:</b>	C12H14N2O2
<b>SMILES:</b>	CC(=O)N1C(=O)C(C)CN1c1ccccc1
<b>Mol. weight [g/mol]:</b>	218.25
<b>CAS:</b>	2655-48-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.82		Crippen Method
logp	1.433		Crippen Method
mcvol	168.420	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=C2655483&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2655483&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

Latest version available from:

<https://www.chemeo.com/cid/117-829-2/1-Phenyl-2-acetyl-4-methyl-3-pyrazolidone.pdf>

Generated by Cheméo on 2024-05-12 21:08:47.822274263 +0000 UTC m=+17837376.742851575.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.