

# 1-Phenyl-4,4-dimethyl-3-pyrazolidone

<b>Other names:</b>	4,4-dimethyl-1-phenyl-3-pyrazolidone
<b>Inchi:</b>	InChI=1S/C11H14N2O/c1-11(2)8-13(12-10(11)14)9-6-4-3-5-7-9/h3-7H,8H2,1-2H3,(H,12,
<b>InchiKey:</b>	SJSJAWHHGDPBOC-UHFFFAOYSA-N
<b>Formula:</b>	C11H14N2O
<b>SMILES:</b>	CC1(C)CN(c2ccccc2)NC1=O
<b>Mol. weight [g/mol]:</b>	190.24
<b>CAS:</b>	2654-58-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	1.564		Crippen Method
mcvol	152.760	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2654582&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2654582&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>
<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

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