

# 2-Pyrazoline-5-one, 4,4-dimethyl-3-isopropyl-1-phenyl-

Inchi:	InChI=1S/C14H18N2O/c1-10(2)12-14(3,4)13(17)16(15-12)11-8-6-5-7-9-11/h5-10H,1-4H3
InchiKey:	OTFORNMJURLTPW-UHFFFAOYSA-N
Formula:	C14H18N2O
SMILES:	CC(C)C1=NN(c2ccccc2)C(=O)C1(C)C
Mol. weight [g/mol]:	230.31
CAS:	92292-40-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	3.071		Crippen Method
mcvol	190.730	ml/mol	McGowan Method

## Sources

McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C92292405&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C92292405&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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