

# 2-Pyrazoline, 5-ethyl-3,5-dimethyl, 1-benzoyl

**Inchi:** InChI=1S/C14H18N2O/c1-4-14(3)10-11(2)15-16(14)13(17)12-8-6-5-7-9-12/h5-9H,4,10H2  
**InchiKey:** SBXDTMIOGHVNGJ-UHFFFAOYSA-N  
**Formula:** C14H18N2O  
**SMILES:** CCC1(C)CC(C)=NN1C(=O)c1ccccc1  
**Mol. weight [g/mol]:** 230.31

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	3.077		Crippen Method
mcvol	190.730	ml/mol	McGowan Method
rinpol	1789.00		NIST Webbook
rinpol	1789.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R322975&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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