

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

<b>Inchi:</b>	InChI=1S/C16H22N2O/c1-4-5-11-14-12-16(2,3)18(17-14)15(19)13-9-7-6-8-10-13/h6-10H
<b>InchiKey:</b>	RIRWHQBPCDUTGP-UHFFFAOYSA-N
<b>Formula:</b>	C16H22N2O
<b>SMILES:</b>	CCCCC1=NN(C(=O)c2ccccc2)C(C)(C)C1
<b>Mol. weight [g/mol]:</b>	258.36

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.71		Crippen Method
logp	3.857		Crippen Method
mcvol	218.910	ml/mol	McGowan Method
rinpola	1935.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R322935&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R322935&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
<b>rinpola:</b>	Non-polar retention indices

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