

# 2-Pyrazoline, 1-isobutyl-3-methyl-

<b>Other names:</b>	3-Methyl-1-isobutyl-«DELTA»[2]-pyrazoline 1-Isobutyl-3-methyl-4,5-dihydro-1H-pyrazole 2-Pyrazoline, 3-methyl-1-(2-methylpropyl)
<b>Inchi:</b>	InChI=1S/C8H16N2/c1-7(2)6-10-5-4-8(3)9-10/h7H,4-6H2,1-3H3
<b>InchiKey:</b>	ZEWMFEJLDHQAFQ-UHFFFAOYSA-N
<b>Formula:</b>	C8H16N2
<b>SMILES:</b>	CC1=NN(CC(C)C)CC1
<b>Mol. weight [g/mol]:</b>	140.23
<b>CAS:</b>	26964-53-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.55		Crippen Method
logp	1.724		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
rinpol	1087.00		NIST Webbook
rinpol	1087.00		NIST Webbook

## Sources

<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=C26964534&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C26964534&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>

## 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>rinpol:</b>	Non-polar retention indices

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