

# Pyrazine, 2-methyl-5-(1-methylethyl)-

<b>Other names:</b>	Pyrazine, 2-isopropyl-5-methyl- 2-Methyl-5-isopropylpyrazine 5-Isopropyl-2-methylpyrazine 2-Isopropyl-5-methylpyrazine 2-Methyl-5-(1-methylethyl)pyrazine
<b>Inchi:</b>	InChI=1S/C8H12N2/c1-6(2)8-5-9-7(3)4-10-8/h4-6H,1-3H3
<b>InchiKey:</b>	PGTQKVQDZHXLOP-UHFFFAOYSA-N
<b>Formula:</b>	C8H12N2
<b>SMILES:</b>	Cc1cnc(C(C)C)cn1
<b>Mol. weight [g/mol]:</b>	136.19
<b>CAS:</b>	13925-05-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	1.908		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
rinpol	1031.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1044.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1403.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1415.00		NIST Webbook
ripol	1400.00		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=C13925058&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13925058&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
<b>ripol:</b>	Polar retention indices

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