

# 2-Methyl-3-isopropylpyrazine

<b>Other names:</b>	3-Isopropyl-2-methylpyrazine Pyrazine, 2-methyl-3-(1-methylethyl) Pyrazine, 2-methyl-3-isopropyl 2-Isopropyl-3-methylpyrazine
<b>Inchi:</b>	InChI=1S/C8H12N2/c1-6(2)8-7(3)9-4-5-10-8/h4-6H,1-3H3
<b>InchiKey:</b>	LNSYLBZKBDNL-UHFFFAOYSA-N
<b>Formula:</b>	C8H12N2
<b>SMILES:</b>	<chem>Cc1nccnc1C(C)C</chem>
<b>Mol. weight [g/mol]:</b>	136.19
<b>CAS:</b>	15986-81-9

## 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	1056.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1025.00		NIST Webbook
ripol	1362.00		NIST Webbook
ripol	1387.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C15986819&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15986819&amp;Units=SI</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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