

# Pyrazine, 2-methoxy-3-(1-methylpropyl)-

<b>Other names:</b>	2-sec-Butyl-3-Methoxypyrazine 2-Methoxy-3-sec-butylpyrazine 2-Methoxy-3-(1-methyl-propyl) pyrazine 3-sec-Butyl-2-methoxypyrazine Pyrazine, 2-methoxy, 3-sec-butyl Pyrazine, 3-methoxy-2-(1-methylpropyl)
<b>Inchi:</b>	InChI=1S/C9H14N2O/c1-4-7(2)8-9(12-3)11-6-5-10-8/h5-7H,4H2,1-3H3
<b>InchiKey:</b>	QMQDJVIJVPEQHE-UHFFFAOYSA-N
<b>Formula:</b>	C9H14N2O
<b>SMILES:</b>	CCC(C)c1nccnc1OC
<b>Mol. weight [g/mol]:</b>	166.22
<b>CAS:</b>	24168-70-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	1.999		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
rinpol	1179.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1159.00		NIST Webbook
ripol	1500.00		NIST Webbook

ripol	1500.00	NIST Webbook
ripol	1494.00	NIST Webbook
ripol	1503.00	NIST Webbook
ripol	1475.00	NIST Webbook
ripol	1490.00	NIST Webbook
ripol	1510.00	NIST Webbook
ripol	1492.00	NIST Webbook
ripol	1503.00	NIST Webbook
ripol	1514.00	NIST Webbook
ripol	1509.00	NIST Webbook

## Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C24168705&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C24168705&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>ripol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices

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