

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

<b>Other names:</b>	2-Isopropyl-3-methoxypyrazine 2-Methoxy-3-isopropylpyrazine 3-Isopropyl-2-methoxypyrazine
<b>Inchi:</b>	InChI=1S/C8H12N2O/c1-6(2)7-8(11-3)10-5-4-9-7/h4-6H,1-3H3
<b>InchiKey:</b>	NTOPKICPEQUPPH-UHFFFAOYSA-N
<b>Formula:</b>	C8H12N2O
<b>SMILES:</b>	COc1nccnc1C(C)C
<b>Mol. weight [g/mol]:</b>	152.19
<b>CAS:</b>	25773-40-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	1.609		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
rinpol	1098.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1096.00		NIST Webbook

rinpol	1098.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1076.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1083.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1078.00	NIST Webbook
rinpol	1078.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1078.00	NIST Webbook
rinpol	1096.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1089.00	NIST Webbook
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rinpol	1093.00	NIST Webbook
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ripol	1434.00	NIST Webbook
ripol	1425.00	NIST Webbook
ripol	1427.00	NIST Webbook
ripol	1413.00	NIST Webbook
ripol	1419.00	NIST Webbook
ripol	1420.00	NIST Webbook
ripol	1461.00	NIST Webbook
ripol	1443.00	NIST Webbook

ripol	1444.00	NIST Webbook
ripol	1465.00	NIST Webbook
ripol	1475.00	NIST Webbook
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ripol	1400.00	NIST Webbook
ripol	1410.00	NIST Webbook
ripol	1400.00	NIST Webbook
ripol	1410.00	NIST Webbook
ripol	1432.00	NIST Webbook
ripol	1429.00	NIST Webbook
ripol	1400.00	NIST Webbook
ripol	1445.00	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=C25773404&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C25773404&amp;Units=SI</a>
<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>

# 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
<b>ripola:</b>	Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/38-129-7/Pyrazine-2-methoxy-3-1-methylethyl.pdf>

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