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

Other names:	2-Isobutyl-3-methoxypyrazine
	2-Methoxy-3-isobutylpyrazine
	2-Methoxy-3-(2-methyl-propyl) pyrazine
	3-Isobutyl-2-methoxypyrazine
	3-Methoxy-2-isobutylpyrazine
	Pyrazine, 2-(2-methylpropyl)-3-methoxy
	Pyrazine, 2-isobutyl-3-methoxy
	Pyrazine, 2-methoxy, 3-isobutyl
	Pyrazine, 3-methoxy-2-(2-methylpropyl)
Inchi:	InChI=1S/C9H14N2O/c1-7(2)6-8-9(12-3)11-5-4-10-8/h4-5,7H,6H2,1-3H3
InchiKey:	UXFSPRAGHGMRSQ-UHFFFAOYSA-N
Formula:	C9H14N2O
SMILES:	COc1nccnc1CC(C)C
Mol. weight [g/mol]:	166.22
CAS:	24683-00-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	1.684		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
rinpol	1161.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1184.00		NIST Webbook

rinpol	1184.00	NIST Webbook
rinpol	1175.00	NIST Webbook
rinpol	1178.00	NIST Webbook
rinpol	1187.00	NIST Webbook
rinpol	1186.00	NIST Webbook
rinpol	1173.00	NIST Webbook
rinpol	1163.00	NIST Webbook
rinpol	1183.00	NIST Webbook
rinpol	1174.00	NIST Webbook
rinpol	1184.00	NIST Webbook
rinpol	1195.00	NIST Webbook
rinpol	1195.00	NIST Webbook
rinpol	1160.00	NIST Webbook
rinpol	1211.00	NIST Webbook
rinpol	1175.00	NIST Webbook
rinpol	1161.00	NIST Webbook
rinpol	1161.00	NIST Webbook
rinpol	1185.00	NIST Webbook
rinpol	1166.00	NIST Webbook
rinpol	1184.00	NIST Webbook
rinpol	1179.00	NIST Webbook
rinpol	1183.00	NIST Webbook
rinpol	1193.00	NIST Webbook
rinpol	1156.00	NIST Webbook
rinpol	1184.00	NIST Webbook
rinpol	1175.00	NIST Webbook
rinpol	1181.00	NIST Webbook
rinpol	1185.00	NIST Webbook
rinpol	1187.00	NIST Webbook
rinpol	1176.00	NIST Webbook
rinpol	1186.00	NIST Webbook
rinpol	1187.00	NIST Webbook
rinpol	1186.00	NIST Webbook
rinpol	1181.00	NIST Webbook
rinpol	1164.00	NIST Webbook
rinpol	1181.00	NIST Webbook
rinpol	1186.00	NIST Webbook
rinpol	1175.00	NIST Webbook
rinpol	1163.00	NIST Webbook
rinpol	1195.00	NIST Webbook
rinpol	1180.00	NIST Webbook
ripol	1511.00	NIST Webbook
ripol	1520.00	NIST Webbook
ripol	1512.00	NIST Webbook

ripol	1558.00	NIST Webbook
ripol	1494.00	NIST Webbook
ripol	1523.00	NIST Webbook
ripol	1527.00	NIST Webbook
ripol	1535.00	NIST Webbook
ripol	1537.00	NIST Webbook
ripol	1514.00	NIST Webbook
ripol	1529.00	NIST Webbook
ripol	1515.00	NIST Webbook
ripol	1514.00	NIST Webbook
ripol	1519.00	NIST Webbook
ripol	1517.00	NIST Webbook
ripol	1517.00	NIST Webbook
ripol	1517.00	NIST Webbook
ripol	1513.00	NIST Webbook
ripol	1525.00	NIST Webbook
ripol	1529.00	NIST Webbook
ripol	1540.00	NIST Webbook
ripol	1531.00	NIST Webbook
ripol	1510.00	NIST Webbook
ripol	1545.00	NIST Webbook
ripol	1549.00	NIST Webbook
ripol	1529.00	NIST Webbook
ripol	1514.00	NIST Webbook
ripol	1545.00	NIST Webbook
ripol	1506.00	NIST Webbook
ripol	1516.00	NIST Webbook
ripol	1525.00	NIST Webbook
ripol	1525.00	NIST Webbook
ripol	1500.00	NIST Webbook
ripol	1494.00	NIST Webbook
ripol	1517.00	NIST Webbook
ripol	1517.00	NIST Webbook
ripol	1517.00	NIST Webbook
ripol	1520.00	NIST Webbook
ripol	1519.00	NIST Webbook
ripol	1521.00	NIST Webbook
ripol	1510.00	NIST Webbook
ripol	1510.00	NIST Webbook
ripol	1511.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24683009&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

Latest version available from:

https://www.chemeo.com/cid/22-852-1/Pyrazine-2-methoxy-3-2-methylpropyl.pdf

Generated by Cheméo on 2024-10-12 04:11:48.46657124 +0000 UTC m=+3287171.103540497.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.