

Pyrazine, 2-chloro-3-methyl-

Other names:	2-Chloro-3-methylpyrazine 2-Methyl-3-chloropyrazine 3-Chloro-2-methyl pyrazine
Inchi:	InChI=1S/C5H5ClN2/c1-4-5(6)8-3-2-7-4/h2-3H,1H3
InchiKey:	WZHWPZQQPWKEAV-UHFFFAOYSA-N
Formula:	C5H5ClN2
SMILES:	Cc1nccnc1Cl
Mol. weight [g/mol]:	128.56
CAS:	95-58-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.16		Crippen Method
logp	1.438		Crippen Method
mcvol	89.750	ml/mol	McGowan Method
rinpol	951.00		NIST Webbook
rinpol	951.00		NIST Webbook
ripol	1399.00		NIST Webbook
ripol	1399.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95589&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/40-620-8/Pyrazine-2-chloro-3-methyl.pdf>

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