

# 3-Chloro-2,5-dimethylpyrazine

<b>Other names:</b>	Pyrazine, 3-chloro-2,5-dimethyl- 2-Chloro-3,6-dimethylpyrazine
<b>Inchi:</b>	InChI=1S/C6H7ClN2/c1-4-3-8-5(2)6(7)9-4/h3H,1-2H3
<b>InchiKey:</b>	NNBALVIZMGWZHS-UHFFFAOYSA-N
<b>Formula:</b>	C6H7ClN2
<b>SMILES:</b>	<chem>Cc1cnc(C)c(Cl)n1</chem>
<b>Mol. weight [g/mol]:</b>	142.59
<b>CAS:</b>	95-89-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Crippen Method
logp	1.747		Crippen Method
mcvol	103.840	ml/mol	McGowan Method
rinpol	1128.00		NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	340.70	K	1.00	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=C95896&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C95896&amp;Units=SI</a>
<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.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>rinpol:</b>	Non-polar retention indices
<b>tbrp:</b>	Boiling point at reduced pressure

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