

# Pyrazine, 2-chloro-3-methyl-5-(2-methylbutyl)

**Other names:** 2-chloro-3-methyl-5-(2-methylbutyl)pyrazine  
**Inchi:** InChI=1S/C10H15ClN2/c1-4-7(2)5-9-6-12-10(11)8(3)13-9/h6-7H,4-5H2,1-3H3  
**InchiKey:** ZAWXZNXSZNHJGO-UHFFFAOYSA-N  
**Formula:** C10H15ClN2  
**SMILES:** CCC(C)Cc1cnc(Cl)c(C)n1  
**Mol. weight [g/mol]:** 198.69

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	3.027		Crippen Method
mcvol	160.200	ml/mol	McGowan Method
rinpol	1371.00		NIST Webbook
rinpol	1371.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1710.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R38274&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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

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