

# Pyrazine, 2,3-dimethyl-5-(2-methylbutyl)

**Other names:** 2,3-dimethyl-5-(2-methylbutyl)pyrazine  
**Inchi:** InChI=1S/C11H18N2/c1-5-8(2)6-11-7-12-9(3)10(4)13-11/h7-8H,5-6H2,1-4H3  
**InchiKey:** QJQUDEDFDDMKGC-UHFFFAOYSA-N  
**Formula:** C11H18N2  
**SMILES:** CCC(C)Cc1cnc(C)c(C)n1  
**Mol. weight [g/mol]:** 178.27

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	2.682		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
rinpol	1306.00		NIST Webbook
ripol	1636.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R38210&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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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