

# 2-isobutyl-6-methylpyrazine

**Other names:** Pyrazine, 6-methyl-2-(2-methylpropyl)  
**Inchi:** InChI=1S/C9H14N2/c1-7(2)4-9-6-10-5-8(3)11-9/h5-7H,4H2,1-3H3  
**InchiKey:** LIRDEXCRJBABIY-UHFFFAOYSA-N  
**Formula:** C9H14N2  
**SMILES:** Cc1cncc(CC(C)C)n1  
**Mol. weight [g/mol]:** 150.22

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	1.984		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
ripol	1495.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1495.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R266414&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)  
**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  
**ripol:** Polar retention indices

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