

# 2-methyl-5-butylpyrazine

<b>Inchi:</b>	InChI=1S/C9H14N2/c1-3-4-5-9-7-10-8(2)6-11-9/h6-7H,3-5H2,1-2H3
<b>InchiKey:</b>	ICMOJSQWNJQRQI-UHFFFAOYSA-N
<b>Formula:</b>	C9H14N2
<b>SMILES:</b>	CCCCc1cnc(C)cn1
<b>Mol. weight [g/mol]:</b>	150.22

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	2.128		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1114.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R219735&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R219735&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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

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