

# 2-Chloro-3-(3,6-dimethyl-2-pyrazyl methyl)-6-methyl pyrazine

<b>Inchi:</b>	InChI=1S/C12H13ClN4/c1-7-5-14-9(3)10(16-7)4-11-12(13)17-8(2)6-15-11/h5-6H,4H2,1-3
<b>InchiKey:</b>	DHIFZEKWXFBNFZ-UHFFFAOYSA-N
<b>Formula:</b>	C12H13ClN4
<b>SMILES:</b>	<chem>Cc1cnc(Cc2nc(C)cnc2C)c(Cl)n1</chem>
<b>Mol. weight [g/mol]:</b>	248.71
<b>CAS:</b>	116374-07-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.75		Crippen Method
logp	2.436		Crippen Method
mcvol	184.580	ml/mol	McGowan Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116374073&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116374073&amp;Units=SI</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

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