

# 2-(N-n-hexylamino)-3,6-dimethyl pyrazine

<b>Inchi:</b>	InChI=1S/C12H21N3/c1-4-5-6-7-8-13-12-11(3)14-9-10(2)15-12/h9H,4-8H2,1-3H3,(H,13,
<b>InchiKey:</b>	PUUVJTVHJVLXCG-UHFFFAOYSA-N
<b>Formula:</b>	C12H21N3
<b>SMILES:</b>	CCCCCNc1nc(C)cnc1C
<b>Mol. weight [g/mol]:</b>	207.32
<b>CAS:</b>	13134-55-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.06		Crippen Method
logp	3.086		Crippen Method
mcvol	186.120	ml/mol	McGowan Method

## Sources

<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=C13134559&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13134559&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>

## 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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