

# 2-(N-n-hexylamino)-3-methyl pyrazine

<b>Inchi:</b>	InChI=1S/C11H19N3/c1-3-4-5-6-7-13-11-10(2)12-8-9-14-11/h8-9H,3-7H2,1-2H3,(H,13,14)
<b>InchiKey:</b>	ROKCGUDSXKFEIO-UHFFFAOYSA-N
<b>Formula:</b>	C11H19N3
<b>SMILES:</b>	CCCCCNc1nccnc1C
<b>Mol. weight [g/mol]:</b>	193.29
<b>CAS:</b>	116660-37-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.58		Crippen Method
logp	2.777		Crippen Method
mcvol	172.030	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=C116660378&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660378&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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