

# 2-Phenoxy-3,6-dimethyl pyrazine

<b>Inchi:</b>	InChI=1S/C12H12N2O/c1-9-8-13-10(2)12(14-9)15-11-6-4-3-5-7-11/h3-8H,1-2H3
<b>InchiKey:</b>	XHMYGFGJEP COIE-UHFFFAOYSA-N
<b>Formula:</b>	C12H12N2O
<b>SMILES:</b>	Cc1cnc(C)c(Oc2ccccc2)n1
<b>Mol. weight [g/mol]:</b>	200.24
<b>CAS:</b>	116660-24-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.886		Crippen Method
mcvol	158.250	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660243&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660243&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

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