

# 3-(P-phenylphenoxy)-2,5-dimethyl pyrazine

<b>Inchi:</b>	InChI=1S/C18H16N2O/c1-13-12-19-14(2)18(20-13)21-17-10-8-16(9-11-17)15-6-4-3-5-7-
<b>InchiKey:</b>	IBXDCIKMQLCFNL-UHFFFAOYSA-N
<b>Formula:</b>	C18H16N2O
<b>SMILES:</b>	Cc1cnc(C)c(Oc2ccc(-c3ccccc3)cc2)n1
<b>Mol. weight [g/mol]:</b>	276.33
<b>CAS:</b>	116660-20-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.19		Crippen Method
logp	4.553		Crippen Method
mcvol	219.030	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=C116660209&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660209&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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