

# 3-(P-t-butylphenoxy)-2,5-dimethyl pyrazine

<b>Inchi:</b>	InChI=1S/C16H20N2O/c1-11-10-17-12(2)15(18-11)19-14-8-6-13(7-9-14)16(3,4)5/h6-10H
<b>InchiKey:</b>	SZJTXDUFOSJTMM-UHFFFAOYSA-N
<b>Formula:</b>	C16H20N2O
<b>SMILES:</b>	Cc1cnc(C)c(Oc2ccc(C(C)(C)C)cc2)n1
<b>Mol. weight [g/mol]:</b>	256.34
<b>CAS:</b>	116660-13-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.90		Crippen Method
logp	4.183		Crippen Method
mcvol	214.610	ml/mol	McGowan Method

## Sources

<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=C116660130&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660130&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>

## 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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