

# 2-(P-nonylphenoxy)-3-methyl-6-(5-nonyl)pyrazine

<b>Inchi:</b>	InChI=1S/C29H46N2O/c1-5-8-11-12-13-14-15-16-25-19-21-27(22-20-25)32-29-24(4)30-
<b>InchiKey:</b>	ZNUOKLVLLDFYRI-UHFFFAOYSA-N
<b>Formula:</b>	C29H46N2O
<b>SMILES:</b>	CCCCCCCCc1ccc(Oc2nc(C(CCCC)CCCC)cnc2C)cc1
<b>Mol. weight [g/mol]:</b>	438.69
<b>CAS:</b>	116402-96-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-10.54		Crippen Method
logp	9.334		Crippen Method
mcvol	397.780	ml/mol	McGowan Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402961&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402961&amp;Units=SI</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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