

# 2-(P-nonylphenoxy)-3-benzyl pyrazine

<b>Inchi:</b>	InChI=1S/C26H32N2O/c1-2-3-4-5-6-7-9-12-22-15-17-24(18-16-22)29-26-25(27-19-20-28
<b>InchiKey:</b>	SZICRUMYIVYVSD-UHFFFAOYSA-N
<b>Formula:</b>	C26H32N2O
<b>SMILES:</b>	CCCCCCCCc1ccc(Oc2nccnc2Cc2ccccc2)cc1
<b>Mol. weight [g/mol]:</b>	388.55
<b>CAS:</b>	116660-03-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.47		Crippen Method
logp	7.153		Crippen Method
mcvol	331.750	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=C116660038&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660038&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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