

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

<b>Inchi:</b>	InChI=1S/C27H34N2O/c1-2-3-4-5-6-7-9-14-24-15-18-25(19-16-24)30-27-26(28-21-22-29
<b>InchiKey:</b>	DPIKCIFLVRQVPG-UHFFFAOYSA-N
<b>Formula:</b>	C27H34N2O
<b>SMILES:</b>	CCCCCCCCc1ccc(Oc2nccnc2CCc2ccccc2)cc1
<b>Mol. weight [g/mol]:</b>	402.57
<b>CAS:</b>	116402-94-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.79		Crippen Method
logp	7.347		Crippen Method
mcvol	345.840	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=C116402949&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402949&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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

Latest version available from:

<https://www.chemeo.com/cid/86-391-3/2-P-nonylphenoxy-3-2-phenylethyl-pyrazine.pdf>

Generated by Cheméo on 2024-04-20 09:24:55.510234356 +0000 UTC m=+15894344.430811668.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.