

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

Inchi:	InChI=1S/C33H54N2O/c1-5-9-13-14-15-16-18-19-28-23-25-30(26-24-28)36-33-31(22-17
InchiKey:	VPKTYKKCTNBEGU-UHFFFAOYSA-N
Formula:	C33H54N2O
SMILES:	CCCCCCCCCc1ccc(Oc2nc(C(CCCC)CCCC)cnc2CCCC)cc1
Mol. weight [g/mol]:	494.79
CAS:	116402-98-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-12.13		Crippen Method
logp	10.759		Crippen Method
mcvol	454.140	ml/mol	McGowan Method

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402983&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402983&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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