

2-(P-nonylphenoxy)-3-n-pentyl pyrazine

Inchi:	InChI=1S/C24H36N2O/c1-3-5-7-8-9-10-12-13-21-15-17-22(18-16-21)27-24-23(14-11-6-4
InchiKey:	JHWFXFCHLCBBGO-UHFFFAOYSA-N
Formula:	C24H36N2O
SMILES:	CCCCCCCCCc1ccc(Oc2nccnc2CCCC)cc1
Mol. weight [g/mol]:	368.56
CAS:	116659-79-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.43		Crippen Method
logp	7.295		Crippen Method
mcvol	327.330	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116659791&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/42-100-3/2-P-nonylphenoxy-3-n-pentyl-pyrazine.pdf>

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