

2-(P-nonylphenoxy)-3,6-dimethyl pyrazine

Inchi:	InChI=1S/C21H30N2O/c1-4-5-6-7-8-9-10-11-19-12-14-20(15-13-19)24-21-18(3)22-16-17
InchiKey:	VGRZBOZMQBSNEV-UHFFFAOYSA-N
Formula:	C21H30N2O
SMILES:	CCCCCCCCCc1ccc(Oc2nc(C)cnc2C)cc1
Mol. weight [g/mol]:	326.48
CAS:	116660-22-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.32		Crippen Method
logp	6.179		Crippen Method
mcvol	285.060	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660221&Units=SI

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/32-766-6/2-P-nonylphenoxy-3-6-dimethyl-pyrazine.pdf>

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