

2-(P-nonylphenoxy)-3-methyl pyrazine

Inchi:	InChI=1S/C20H28N2O/c1-3-4-5-6-7-8-9-10-18-11-13-19(14-12-18)23-20-17(2)21-15-16-
InchiKey:	MIFCXYCKDIHAKQ-UHFFFAOYSA-N
Formula:	C20H28N2O
SMILES:	CCCCCCCCc1ccc(Oc2nccnc2C)cc1
Mol. weight [g/mol]:	312.45
CAS:	116660-49-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.85		Crippen Method
logp	5.870		Crippen Method
mcvol	270.970	ml/mol	McGowan Method

Sources

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=C116660492&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/96-475-9/2-P-nonylphenoxy-3-methyl-pyrazine.pdf>

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