

2-(O-phenylphenoxy)-3,6-dimethyl pyrazine

Inchi:	InChI=1S/C18H16N2O/c1-13-12-19-14(2)18(20-13)21-17-11-7-6-10-16(17)15-8-4-3-5-9-
InchiKey:	YZZJKVRKCKCCIJ-UHFFFAOYSA-N
Formula:	C18H16N2O
SMILES:	Cc1cnc(C)c(Oc2ccccc2-c2ccccc2)n1
Mol. weight [g/mol]:	276.33
CAS:	116660-25-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.19		Crippen Method
logp	4.553		Crippen Method
mcvol	219.030	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=C116660254&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/26-733-9/2-O-phenylphenoxy-3-6-dimethyl-pyrazine.pdf>

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