

2-(M-phenoxyphenoxy)-3-methyl pyrazine

Inchi:	InChI=1S/C17H14N2O2/c1-13-17(19-11-10-18-13)21-16-9-5-8-15(12-16)20-14-6-3-2-4-7
InchiKey:	XHCRKXJKKOSJPJ-UHFFFAOYSA-N
Formula:	C17H14N2O2
SMILES:	Cc1nccnc1Oc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]:	278.31
CAS:	116659-73-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.75		Crippen Method
logp	4.370		Crippen Method
mcvol	210.810	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C116659735&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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