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/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=C116659735&Units=SI

Legend

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