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