2-(O-phenylphenoxy)-3-methyl pyrazine

Inchi: InChI=1S/C17H14N2O/c1-13-17(19-12-11-18-13)20-16-10-6-5-9-15(16)14-7-3-2-4-8-14/h
InchiKey: USLZXOBENXPOCF-UHFFFAOYSA-N
Formula: C17H14N2O
SMILES: Cc1nccnc1Oc1ccccc1-c1ccccc1
Mol. weight [g/mol]: 262.31
CAS: 93323-45-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.72		Crippen Method
logp	4.244		Crippen Method
mcvol	204.940	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C93323456&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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