2-(O-phenylphenoxy) pyrazine

Inchi: InChI=1S/C16H12N2O/c1-2-6-13(7-3-1)14-8-4-5-9-15(14)19-16-12-17-10-11-18-16/h1-12
InchiKey: CHFDNBAZVGQWTL-UHFFFAOYSA-N
Formula: C16H12N2O
SMILES: c1ccc(-c2ccccc2Oc2cnccn2)cc1
Mol. weight [g/mol]: 248.28
CAS: 116435-19-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.24		Crippen Method
logp	3.936		Crippen Method
mcvol	190.850	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=C116435199&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