2-(P-t-butylphenoxy)-3-(2-phenylethyl) pyrazine

Inchi: InChI=1S/C22H24N2O/c1-22(2,3)18-10-12-19(13-11-18)25-21-20(23-15-16-24-21)14-9-1

InchiKey: QNYYJZCDAPBEPI-UHFFFAOYSA-N

Formula: C22H24N2O

SMILES: CC(C)(C)c1ccc(Oc2nccnc2CCc2ccccc2)cc1

Mol. weight [g/mol]: 332.44

CAS: 116295-59-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.37		Crippen Method
logp	5.352		Crippen Method
mcvol	275.390	ml/mol	McGowan Method

Sources

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=C116295591&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume