

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

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<https://www.chemeo.com/cid/53-710-4/2-P-t-butylphenoxy-3-2-phenylethyl-pyrazine.pdf>

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