2-(P-methylphenoxy)-3-methyl pyrazine

Inchi: InChI=1S/C12H12N2O/c1-9-3-5-11(6-4-9)15-12-10(2)13-7-8-14-12/h3-8H,1-2H3
InchiKey: VFXFVQJLZMZESR-UHFFFAOYSA-N
Formula: C12H12N2O
SMILES: Cc1ccc(Oc2nccnc2C)cc1
Mol. weight [g/mol]: 200.24
CAS: 91392-06-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.886		Crippen Method
mcvol	158.250	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=C91392062&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