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

Inchi: InChI=1S/C15H18N2O/c1-11-14(17-10-9-16-11)18-13-7-5-12(6-8-13)15(2,3)4/h5-10H,1-
InchiKey: QSRAWVAHHWVLRU-UHFFFAOYSA-N
Formula: C15H18N2O
SMILES: Cc1nccnc1Oc1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 242.32
CAS: 116660-14-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.43		Crippen Method
logp	3.875		Crippen Method
mcvol	200.520	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660141&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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