2-(O-isopropylphenoxy)-3-methyl pyrazine

Inchi: InChI=1S/C14H16N2O/c1-10(2)12-6-4-5-7-13(12)17-14-11(3)15-8-9-16-14/h4-10H,1-3H
InchiKey: CZGWVSUJMLUQBW-UHFFFAOYSA-N
Formula: C14H16N2O
SMILES: Cc1nccnc1Oc1ccccc1C(C)C
Mol. weight [g/mol]: 228.29
CAS: 116660-40-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.30		Crippen Method
logp	3.701		Crippen Method
mcvol	186.430	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=C116660403&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