2-(2-Methyl-6-ethylphenoxy)-3-methyl pyrazine

Inchi: InChI=1S/C14H16N2O/c1-4-12-7-5-6-10(2)13(12)17-14-11(3)15-8-9-16-14/h5-9H,4H2,1-
InchiKey: LRCSDHFIKKCFNX-UHFFFAOYSA-N
Formula: C14H16N2O
SMILES: CCc1cccc(C)c1Oc1nccnc1C
Mol. weight [g/mol]: 228.29
CAS: 116660-46-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	3.448		Crippen Method
mcvol	186.430	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660469&Units=SI

Legend

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