2-(M-methoxyphenoxy)-3-methyl pyrazine

Inchi: InChI=1S/C12H12N2O2/c1-9-12(14-7-6-13-9)16-11-5-3-4-10(8-11)15-2/h3-8H,1-2H3
InchiKey: QOGDMTJYROWOSQ-UHFFFAOYSA-N
Formula: C12H12N2O2
SMILES: COc1cccc(Oc2nccnc2C)c1
Mol. weight [g/mol]: 216.24
CAS: 116660-43-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	2.586		Crippen Method
mcvol	164.120	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=C116660436&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