

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

Inchi: InChI=1S/C12H12N2O/c1-9-4-3-5-11(8-9)15-12-10(2)13-6-7-14-12/h3-8H,1-2H3
InchiKey: KOLCCMRFXREORH-UHFFFAOYSA-N
Formula: C12H12N2O
SMILES: Cc1cccc(Oc2nccnc2C)c1
Mol. weight [g/mol]: 200.24
CAS: 92576-03-9

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C92576039&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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<https://www.chemeo.com/cid/85-622-7/2-M-methylphenoxy-3-methyl-pyrazine.pdf>

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