2-(M-carbomethoxy phenoxy)-3-methyl pyrazine

Inchi: InChI=1S/C13H12N2O3/c1-9-12(15-7-6-14-9)18-11-5-3-4-10(8-11)13(16)17-2/h3-8H,1-2

InchiKey: WMFJWECHKAUSLG-UHFFFAOYSA-N

Formula: C13H12N2O3

SMILES: COC(=O)c1cccc(Oc2nccnc2C)c1

Mol. weight [g/mol]: 244.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Crippen Method
logp	2.364		Crippen Method
mcvol	179.780	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=B6003290&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