

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/ci9903071

Legend

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

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