

2-(M-methoxy phenoxy) pyrazine

Inchi: InChI=1S/C11H10N2O2/c1-14-9-3-2-4-10(7-9)15-11-8-12-5-6-13-11/h2-8H,1H3
InchiKey: BIFCNYQIWFGULS-UHFFFAOYSA-N
Formula: C11H10N2O2
SMILES: COc1cccc(Oc2cnccn2)c1
Mol. weight [g/mol]: 202.21
CAS: 116660-42-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.76		Crippen Method
logp	2.277		Crippen Method
mcvol	150.030	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660425&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/120-258-2/2-M-methoxy-phenoxy-pyrazine.pdf>

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