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

Inchi: InChI=1S/C11H11N3O/c1-8-11(14-6-5-13-8)15-10-4-2-3-9(12)7-10/h2-7H,12H2,1H3
InchiKey: SLURIHKDPIRKIW-UHFFFAOYSA-N
Formula: C11H11N3O
SMILES: Cc1nccnc1Oc1cccc(N)c1
Mol. weight [g/mol]: 201.22
CAS: 116659-95-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	2.160		Crippen Method
mcvol	154.140	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C116659951&Units=SI

Legend

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

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