

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:	<chem>Cc1nccnc1Oc1cccc(N)c1</chem>
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:	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
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

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