

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

Inchi:	InChI=1S/C11H10N2O2/c1-8-11(13-6-5-12-8)15-10-4-2-3-9(14)7-10/h2-7,14H,1H3
InchiKey:	DXALOKLBXCDATQ-UHFFFAOYSA-N
Formula:	C11H10N2O2
SMILES:	Cc1nccnc1Oc1cccc(O)c1
Mol. weight [g/mol]:	202.21
CAS:	95390-42-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	2.283		Crippen Method
mcvol	150.030	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C95390424&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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<https://www.chemeo.com/cid/113-016-8/2-M-hydroxyphenoxy-3-methyl-pyrazine.pdf>

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