

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

Inchi:	InChI=1S/C12H12N2O2/c1-9-12(14-7-6-13-9)16-11-5-3-4-10(8-11)15-2/h3-8H,1-2H3
InchiKey:	QOGDMTJYROWOSQ-UHFFFAOYSA-N
Formula:	C12H12N2O2
SMILES:	COc1cccc(Oc2nccnc2C)c1
Mol. weight [g/mol]:	216.24
CAS:	116660-43-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	2.586		Crippen Method
mcvol	164.120	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=C116660436&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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<https://www.chemeo.com/cid/50-669-4/2-M-methoxyphenoxy-3-methyl-pyrazine.pdf>

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