

2-(O-isopropylphenoxy)-3-methyl pyrazine

Inchi:	InChI=1S/C14H16N2O/c1-10(2)12-6-4-5-7-13(12)17-14-11(3)15-8-9-16-14/h4-10H,1-3H3
InchiKey:	CZGWVSUJMLUQBW-UHFFFAOYSA-N
Formula:	C14H16N2O
SMILES:	<chem>Cc1nccnc1Oc1ccccc1C(C)C</chem>
Mol. weight [g/mol]:	228.29
CAS:	116660-40-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.30		Crippen Method
logp	3.701		Crippen Method
mcvol	186.430	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=C116660403&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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