

5-isopropyl-3-methyl-2-phenoxy pyrazine

Other names:	Pyrazine, 3-methyl-5-(1-methylethyl)-2-phenoxy
Inchi:	InChI=1S/C14H16N2O/c1-10(2)13-9-15-14(11(3)16-13)17-12-7-5-4-6-8-12/h4-10H,1-3H3
InchiKey:	QDHZPSJIZDNGPB-UHFFFAOYSA-N
Formula:	C14H16N2O
SMILES:	<chem>Cc1nc(C(C)C)cnc1Oc1ccccc1</chem>
Mol. weight [g/mol]:	228.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.30		Crippen Method
logp	3.701		Crippen Method
mcvol	186.430	ml/mol	McGowan Method
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
ripol	2114.00		NIST Webbook
ripol	2114.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R38658&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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