Pyrazine, 3-methyl-5-(2-methylpropyl)-2-phenoxy

Other names: 5-isobutyl-3-methyl-2-phenoxypyrazine

Inchi: InChI=1S/C15H18N2O/c1-11(2)9-13-10-16-15(12(3)17-13)18-14-7-5-4-6-8-14/h4-8,10-1

InchiKey: VQFWHEXRDILCNY-UHFFFAOYSA-N

Formula: C15H18N2O

SMILES: Cc1nc(CC(C)C)cnc1Oc1ccccc1

Mol. weight [g/mol]: 242.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.51		Crippen Method
logp	3.776		Crippen Method
mcvol	200.520	ml/mol	McGowan Method
rinpol	1706.00		NIST Webbook
rinpol	1706.00		NIST Webbook
ripol	2209.00		NIST Webbook
ripol	2209.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R38612&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

rinpol: Non-polar retention indices

ripol: Polar retention indices

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