

# Pyrazine, 2-pentyl-3-phenoxy

**Other names:** Pyrazine, 2-pentyl-3-(phenoxy)  
**Inchi:** InChI=1S/C15H18N2O/c1-2-3-5-10-14-15(17-12-11-16-14)18-13-8-6-4-7-9-13/h4,6-9,11-  
**InchiKey:** CVVZUDIKWBFQQX-UHFFFAOYSA-N  
**Formula:** C15H18N2O  
**SMILES:** CCCCCc1nccnc1Oc1ccccc1  
**Mol. weight [g/mol]:** 242.32

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Crippen Method
logp	4.002		Crippen Method
mcvol	200.520	ml/mol	McGowan Method
rinpol	1816.00		NIST Webbook
rinpol	1816.00		NIST Webbook
ripol	2430.00		NIST Webbook
ripol	2430.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R43588&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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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