

# Pyrazine, 2-(4-methylphenyl)-

**Inchi:** InChI=1S/C11H10N2/c1-9-2-4-10(5-3-9)11-8-12-6-7-13-11/h2-8H,1H3  
**InchiKey:** RMFQOVASJJFORN-UHFFFAOYSA-N  
**Formula:** C11H10N2  
**SMILES:** Cc1ccc(-c2cnccn2)cc1  
**Mol. weight [g/mol]:** 170.21

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	2.452		Crippen Method
mcvol	138.290	ml/mol	McGowan Method
rinpol	1654.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U380546&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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

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