

# Pyrrole, 1-(5-methylfurfuryl)

**Other names:** 1-(5-methylfurfuryl)-pyrrole  
**Inchi:** InChI=1S/C10H11NO/c1-9-4-5-10(12-9)8-11-6-2-3-7-11/h2-7H,8H2,1H3  
**InchiKey:** CAHIUMOBCXFSCC-UHFFFAOYSA-N  
**Formula:** C10H11NO  
**SMILES:** Cc1ccc(Cn2cccc2)o1  
**Mol. weight [g/mol]:** 161.20

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.24		Crippen Method
logp	2.438		Crippen Method
mcvol	128.690	ml/mol	McGowan Method
rinpol	1247.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1248.00		NIST Webbook
ripol	1885.00		NIST Webbook
ripol	1885.00		NIST Webbook

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R62403&Units=SI>

## 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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