

# 5-methyl-1(3H)-isobenzofuran

**Inchi:** InChI=1S/C9H8O/c1-7-2-3-8-5-10-6-9(8)4-7/h2-6H,1H3  
**InchiKey:** BJCGCTDHYXCSTL-UHFFFAOYSA-N  
**Formula:** C9H8O  
**SMILES:** Cc1ccc2cocc2c1  
**Mol. weight [g/mol]:** 132.16

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.49		Crippen Method
logp	2.741		Crippen Method
mcvol	104.620	ml/mol	McGowan Method
rinpol	1159.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R216276&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

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