

# 3-formyl-2-methylfuran

**Inchi:** InChI=1S/C6H6O2/c1-5-6(4-7)2-3-8-5/h2-4H,1H3  
**InchiKey:** WBFUBNWKSDINIX-UHFFFAOYSA-N  
**Formula:** C6H6O2  
**SMILES:** Cc1occc1C=O  
**Mol. weight [g/mol]:** 110.11

## Physical Properties

| Property code | Value  | Unit   | Source         |
|---------------|--------|--------|----------------|
| log10ws       | -5.92  |        | Crippen Method |
| logp          | 1.401  |        | Crippen Method |
| mcvol         | 83.380 | ml/mol | McGowan Method |
| rinpol        | 931.00 |        | NIST Webbook   |
| rinpol        | 931.00 |        | NIST Webbook   |
| rinpol        | 936.00 |        | NIST Webbook   |
| rinpol        | 936.00 |        | NIST Webbook   |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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=R495355&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

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