

# 1-(5-methyl-2-furanyl)-2-butanone

**Inchi:** InChI=1S/C9H12O2/c1-3-8(10)6-9-5-4-7(2)11-9/h4-5H,3,6H2,1-2H3  
**InchiKey:** ZPAROSZTOGYLPX-UHFFFAOYSA-N  
**Formula:** C9H12O2  
**SMILES:** CCC(=O)Cc1ccc(C)o1  
**Mol. weight [g/mol]:** 152.19

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.60		Crippen Method
logp	2.110		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
ripol	1641.00		NIST Webbook
ripol	1636.00		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1642.00		NIST Webbook
ripol	1643.00		NIST Webbook
ripol	1647.00		NIST Webbook
ripol	1636.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R491348&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

**ripol:** Polar retention indices

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