

# 6-Methyl-6-(5-methylfuran-2-yl)heptan-2-one

**Inchi:** InChI=1S/C13H20O2/c1-10(14)6-5-9-13(3,4)12-8-7-11(2)15-12/h7-8H,5-6,9H2,1-4H3  
**InchiKey:** CQPPRTJQWXGAGK-UHFFFAOYSA-N  
**Formula:** C13H20O2  
**SMILES:** CC(=O)CCCC(C)(C)c1ccc(C)o1  
**Mol. weight [g/mol]:** 208.30  
**CAS:** 50464-95-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.95		Crippen Method
logp	3.625		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
rinpol	1426.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1426.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C50464954&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)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/83-214-2/6-Methyl-6-5-methylfuran-2-yl-heptan-2-one.pdf>

Generated by Cheméo on 2024-04-20 14:36:47.298473448 +0000 UTC m=+15913056.219050763.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.