

# 2-Furoic acid, 4-methoxy-2-methylbutyl ester

**Inchi:** InChI=1S/C11H16O4/c1-9(5-7-13-2)8-15-11(12)10-4-3-6-14-10/h3-4,6,9H,5,7-8H2,1-2H3  
**InchiKey:** JJEOLVABDZBQCJ-UHFFFAOYSA-N  
**Formula:** C11H16O4  
**SMILES:** COCCC(C)COC(=O)c1ccco1  
**Mol. weight [g/mol]:** 212.24

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -6.39   |        | Crippen Method |
| logp          | 2.109   |        | Crippen Method |
| mcvol         | 165.570 | ml/mol | McGowan Method |
| rinpol        | 1555.00 |        | NIST Webbook   |

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U355173&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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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