

# 3-Furancarboxylic acid, 2-methyl-, methyl ester

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 3-Furoic acid, 2-methyl-, methyl ester<br>Methyl 2-methyl-3-furancarboxylate<br>Methyl 2-methylfuran-3-carboxylate |
| <b>Inchi:</b>               | InChI=1S/C7H8O3/c1-5-6(3-4-10-5)7(8)9-2/h3-4H,1-2H3  |
| <b>InchiKey:</b>            | UVRRIABXNIGUJZ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C7H8O3   |
| <b>SMILES:</b>              | COC(=O)c1ccoc1C  |
| <b>Mol. weight [g/mol]:</b> | 140.14   |
| <b>CAS:</b>                 | 6141-58-8  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -5.92   |        | Crippen Method |
| logp          | 1.375   |        | Crippen Method |
| mcvol         | 103.340 | ml/mol | McGowan Method |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 348.20 | K    | 2.70           | NIST Webbook |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6141588&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6141588&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                   |

# Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |
| <b>tbrp:</b>    | Boiling point at reduced pressure   |

Latest version available from:

<https://www.cheméo.com/cid/69-595-6/3-Furancarboxylic-acid-2-methyl-methyl-ester.pdf>

Generated by Cheméo on 2024-04-26 03:32:32.659675381 +0000 UTC m=+16391601.580252698.

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