# 3-Ethyl-4-methyl-2,5-furandione

**Other names:** 3-Ethyl-4-methyl-2,5-furanedione
**Inchi:** InChI=1S/C7H8O3/c1-3-5-4(2)6(8)10-7(5)9/h3H2,1-2H3
**InchiKey:** ZVUUAOZFEUKPLC-UHFFFAOYSA-N
**Formula:** C7H8O3
**SMILES:** CCC1=C(C)C(=O)OC1=O
**Mol. weight [g/mol]:** 140.14
**CAS:** 3552-33-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -268.28 | kJ/mol | Joback Method |
| hf | -479.55 | kJ/mol | Joback Method |
| hfus | 14.19 | kJ/mol | Joback Method |
| hvap | 46.36 | kJ/mol | Joback Method |
| log10ws | -1.14 | | Crippen Method |
| logp | 0.796 | | Crippen Method |
| mcvol | 103.340 | ml/mol | McGowan Method |
| pc | 3857.88 | kPa | Joback Method |
| ripol | 1777.00 | | NIST Webbook |
| ripol | 1777.00 | | NIST Webbook |
| ripol | 1777.00 | | NIST Webbook |
| tb | 551.22 | K | Joback Method |
| tc | 786.26 | K | Joback Method |
| tf | 372.60 | K | Joback Method |
| vc | 0.391 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 238.44 | J/mol×K | 551.22 | Joback Method |
| cpg | 250.17 | J/mol×K | 590.39 | Joback Method |
| cpg | 261.47 | J/mol×K | 629.57 | Joback Method |
| cpg | 272.28 | J/mol×K | 668.74 | Joback Method |
| cpg | 282.57 | J/mol×K | 707.91 | Joback Method |

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|---|---|---|---|---|
| cpg | 292.28 | J/mol×K | 747.08 | Joback Method |
| cpg | 301.35 | J/mol×K | 786.26 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3552338&Units=SI |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |