# 2(5H)-Furanone, 5-(1-methylethyl)-

| | |
|---|---|
| **Other names:** | 5-Isopropyl-5H-furan-2-one |
| **Inchi:** | InChI=1S/C7H10O2/c1-5(2)6-3-4-7(8)9-6/h3-6H,1-2H3 |
| **InchiKey:** | LWFKYUIZWLTJCA-UHFFFAOYSA-N |
| **Formula:** | C7H10O2 |
| **SMILES:** | CC(C)C1C=CC(=O)O1 |
| **Mol. weight [g/mol]:** | 126.15 |
| **CAS:** | 56767-19-2 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -136.58 | kJ/mol | Joback Method |
| hf | -344.53 | kJ/mol | Joback Method |
| hfus | 13.01 | kJ/mol | Joback Method |
| hvap | 40.09 | kJ/mol | Joback Method |
| log10ws | -1.23 | | Crippen Method |
| logp | 1.124 | | Crippen Method |
| mcvol | 101.770 | ml/mol | McGowan Method |
| pc | 3718.02 | kPa | Joback Method |
| rinpol | 1311.00 | | NIST Webbook |
| tb | 468.33 | K | Joback Method |
| tc | 689.64 | K | Joback Method |
| tf | 260.10 | K | Joback Method |
| vc | 0.377 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 218.87 | J/mol×K | 468.33 | Joback Method |
| cpg | 232.27 | J/mol×K | 505.22 | Joback Method |
| cpg | 245.06 | J/mol×K | 542.10 | Joback Method |
| cpg | 257.22 | J/mol×K | 578.99 | Joback Method |
| cpg | 268.77 | J/mol×K | 615.87 | Joback Method |
| cpg | 279.69 | J/mol×K | 652.76 | Joback Method |
| cpg | 289.99 | J/mol×K | 689.64 | Joback Method |

# Sources

| | |
|---|---|
| **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=C56767192&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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