# FURFURYL FORMATE

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|---|---|
| **Other names:** | 2-Furylmethyl formate |
| | Furfuryl methanoate |
| | 2-Furanmethanol, 2-formate |
| | furan-2-ylmethyl formate |
| **Inchi:** | InChI=1S/C6H6O3/c7-5-8-4-6-2-1-3-9-6/h1-3,5H,4H2 |
| **InchiKey:** | FPRQARNPKWVCNI-UHFFFAOYSA-N |
| **Formula:** | C6H6O3 |
| **SMILES:** | O=COCc1ccco1 |
| **Mol. weight [g/mol]:** | 126.11 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.4567 | | Cheméo Relay (1.0) |
| hf | -344.19 | kJ/mol | Cheméo Relay (1.0) |
| hvap | 51.82 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.95 | eV | Cheméo Relay (1.0) |
| log10ws | -0.77 | | Cheméo Relay (1.0) |
| logp | 0.953 | | Crippen Method |
| mcvol | 89.250 | ml/mol | McGowan Method |
| pc | 4793.60 | kPa | Cheméo Relay (1.0, beta) |
| rinpol | 902.00 | | NIST Webbook |
| rinpol | 875.00 | | NIST Webbook |
| ripol | 1478.00 | | NIST Webbook |
| ripol | 1480.00 | | NIST Webbook |
| ripol | 1519.00 | | NIST Webbook |
| ripol | 1519.00 | | NIST Webbook |
| ripol | 1519.00 | | NIST Webbook |
| ripol | 1497.00 | | NIST Webbook |
| ripol | 1504.00 | | NIST Webbook |
| ripol | 1519.00 | | NIST Webbook |
| ripol | 1472.00 | | NIST Webbook |
| ripol | 1524.00 | | NIST Webbook |
| ripol | 1479.00 | | NIST Webbook |
| ripol | 1479.00 | | NIST Webbook |
| ripol | 1478.00 | | NIST Webbook |
| ripol | 1515.00 | | NIST Webbook |
| ripol | 1472.00 | | NIST Webbook |

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|---|---|---|---|
| ripol | 1497.00 | | NIST Webbook |
| tb | 447.12 | K | Cheméo Relay (1.0) |
| tc | 649.20 | K | Cheméo Relay (1.0) |
| tf | 239.75 | K | Cheméo Relay (1.0) |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C13493975&Units=SI

# Legend

**af:** Acentric Factor
**hf:** Enthalpy of formation at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**ie:** Ionization energy
**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
**ripol:** Polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point