# Formic acid, 2-methylbutyl ester

**Inchi:** InChI=1S/C6H12O2/c1-3-6(2)4-8-5-7/h5-6H,3-4H2,1-2H3
**InchiKey:** DWORILFBIRYUDC-UHFFFAOYSA-N
**Formula:** C6H12O2
**SMILES:** CCC(C)COC=O
**Mol. weight [g/mol]:** 116.16

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -207.32 | kJ/mol | Joback Method |
| hf | -390.25 | kJ/mol | Joback Method |
| hfus | 11.25 | kJ/mol | Joback Method |
| hvap | 37.69 | kJ/mol | Joback Method |
| log10ws | -0.95 | | Crippen Method |
| logp | 1.205 | | Crippen Method |
| mcvol | 102.840 | ml/mol | McGowan Method |
| pc | 3345.11 | kPa | Joback Method |
| rinpol | 805.00 | | NIST Webbook |
| tb | 407.32 | K | Joback Method |
| tc | 583.97 | K | Joback Method |
| tf | 206.61 | K | Joback Method |
| vc | 0.401 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 201.69 | J/mol×K | 407.32 | Joback Method |
| cpg | 211.53 | J/mol×K | 436.76 | Joback Method |
| cpg | 221.04 | J/mol×K | 466.20 | Joback Method |
| cpg | 230.24 | J/mol×K | 495.64 | Joback Method |
| cpg | 239.12 | J/mol×K | 525.08 | Joback Method |
| cpg | 247.68 | J/mol×K | 554.53 | Joback Method |
| cpg | 255.92 | J/mol×K | 583.97 | Joback Method |
| dvisc | 0.0052383 | Pa×s | 206.61 | Joback Method |
| dvisc | 0.0022883 | Pa×s | 240.06 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0012241 | Pa×s | 273.51 | Joback Method |
| dvisc | 0.0007505 | Pa×s | 306.97 | Joback Method |
| dvisc | 0.0005066 | Pa×s | 340.42 | Joback Method |
| dvisc | 0.0003668 | Pa×s | 373.87 | Joback Method |
| dvisc | 0.0002801 | Pa×s | 407.32 | Joback Method |

# Sources

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|---|---|
| **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=U367911&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |