# methyl 3-acetoxybutanoate

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|---|---|
| **Other names:** | methyl 3-acetoxybutyrate |
| | Methyl butanoate, 3-acetoxy |
| | Butanoic acid, 3-(acetyloxy)-, methyl ester |
| **Inchi:** | InChI=1S/C7H12O4/c1-5(11-6(2)8)4-7(9)10-3/h5H,4H2,1-3H3 |
| **InchiKey:** | GSQSJDKJUCRGGT-UHFFFAOYSA-N |
| **Formula:** | C7H12O4 |
| **SMILES:** | COC(=O)CC(C)OC(C)=O |
| **Mol. weight [g/mol]:** | 160.17 |
| **CAS:** | 89422-42-4 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -462.22 | kJ/mol | Joback Method |
| hf | -682.69 | kJ/mol | Joback Method |
| hfus | 15.94 | kJ/mol | Joback Method |
| hvap | 49.10 | kJ/mol | Joback Method |
| log10ws | -0.59 | | Crippen Method |
| logp | 0.501 | | Crippen Method |
| mcvol | 124.370 | ml/mol | McGowan Method |
| pc | 3121.00 | kPa | Joback Method |
| rinpol | 1016.00 | | NIST Webbook |
| rinpol | 1017.00 | | NIST Webbook |
| rinpol | 1010.00 | | NIST Webbook |
| rinpol | 1011.00 | | NIST Webbook |
| ripol | 1530.00 | | NIST Webbook |
| ripol | 1563.00 | | NIST Webbook |
| ripol | 1529.00 | | NIST Webbook |
| ripol | 1535.00 | | NIST Webbook |
| tb | 511.70 | K | Joback Method |
| tc | 701.34 | K | Joback Method |
| tf | 297.97 | K | Joback Method |
| vc | 0.469 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 278.59 | J/mol×K | 511.70 | Joback Method |
| cpg | 328.25 | J/mol×K | 669.73 | Joback Method |
| cpg | 319.13 | J/mol×K | 638.13 | Joback Method |
| cpg | 309.59 | J/mol×K | 606.52 | Joback Method |
| cpg | 299.65 | J/mol×K | 574.91 | Joback Method |
| cpg | 289.32 | J/mol×K | 543.31 | Joback Method |
| cpg | 336.95 | J/mol×K | 701.34 | Joback Method |
| dvisc | 0.0002344 | Pa×s | 511.70 | Joback Method |
| dvisc | 0.0003024 | Pa×s | 476.08 | Joback Method |
| dvisc | 0.0004067 | Pa×s | 440.46 | Joback Method |
| dvisc | 0.0005762 | Pa×s | 404.84 | Joback Method |
| dvisc | 0.0008732 | Pa×s | 369.21 | Joback Method |
| dvisc | 0.0014459 | Pa×s | 333.59 | Joback Method |
| dvisc | 0.0027013 | Pa×s | 297.97 | Joback Method |

# Sources

**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=C89422424&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

**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

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|---|---|
| **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 |
| **vc:** | Critical Volume |