# 2-acetoxypropanal

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|---|---|
| **Other names:** | 1-formylethyl acetate |
| | Propanal, 2-(acetyloxy)- |
| **Inchi:** | InChI=1S/C5H8O3/c1-4(3-6)8-5(2)7/h3-4H,1-2H3 |
| **InchiKey:** | FXPPNKAYSGWCQG-UHFFFAOYSA-N |
| **Formula:** | C5H8O3 |
| **SMILES:** | CC(=O)OC(C)C=O |
| **Mol. weight [g/mol]:** | 116.12 |
| **CAS:** | 22094-23-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -344.66 | kJ/mol | Joback Method |
| hf | -482.19 | kJ/mol | Joback Method |
| hfus | 10.26 | kJ/mol | Joback Method |
| hvap | 42.21 | kJ/mol | Joback Method |
| log10ws | -0.17 | | Crippen Method |
| logp | 0.137 | | Crippen Method |
| mcvol | 90.320 | ml/mol | McGowan Method |
| pc | 4056.96 | kPa | Joback Method |
| ripol | 1355.00 | | NIST Webbook |
| tb | 438.31 | K | Joback Method |
| tc | 628.27 | K | Joback Method |
| tf | 245.27 | K | Joback Method |
| vc | 0.350 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 178.67 | J/mol×K | 438.31 | Joback Method |
| cpg | 186.67 | J/mol×K | 469.97 | Joback Method |
| cpg | 194.39 | J/mol×K | 501.63 | Joback Method |
| cpg | 201.82 | J/mol×K | 533.29 | Joback Method |
| cpg | 208.97 | J/mol×K | 564.95 | Joback Method |
| cpg | 215.82 | J/mol×K | 596.61 | Joback Method |

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|---|---|---|---|---|
| cpg | 222.38 | J/mol×K | 628.27 | Joback Method |
| dvisc | 0.0040015 | Pa×s | 245.27 | Joback Method |
| dvisc | 0.0020839 | Pa×s | 277.44 | Joback Method |
| dvisc | 0.0012428 | Pa×s | 309.62 | Joback Method |
| dvisc | 0.0008170 | Pa×s | 341.79 | Joback Method |
| dvisc | 0.0005772 | Pa×s | 373.96 | Joback Method |
| dvisc | 0.0004309 | Pa×s | 406.14 | Joback Method |
| dvisc | 0.0003358 | Pa×s | 438.31 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 326.50 ± 1.50 | K | 2.00 | NIST Webbook |

# 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=C22094231&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
**mcvol:** McGowan's characteristic volume
**pc:** Critical Pressure
**ripol:** Polar retention indices

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|---|---|
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |