# Acetoxyacetic acid, (4-chlorophenyl)methyl ester

**Inchi:** InChI=1S/C11H11ClO4/c1-8(13)15-7-11(14)16-6-9-2-4-10(12)5-3-9/h2-5H,6-7H2,1H3
**InchiKey:** IUAPHMNPPYPAAC-UHFFFAOYSA-N
**Formula:** C11H11ClO4
**SMILES:** CC(=O)OCC(=O)OCc1ccc(Cl)cc1
**Mol. weight [g/mol]:** 242.66

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -335.25 | kJ/mol | Joback Method |
| hf | -550.65 | kJ/mol | Joback Method |
| hfus | 27.67 | kJ/mol | Joback Method |
| hvap | 65.72 | kJ/mol | Joback Method |
| log10ws | -2.44 | | Crippen Method |
| logp | 1.946 | | Crippen Method |
| mcvol | 169.210 | ml/mol | McGowan Method |
| pc | 2761.36 | kPa | Joback Method |
| rinpol | 1663.00 | | NIST Webbook |
| tb | 672.75 | K | Joback Method |
| tc | 891.35 | K | Joback Method |
| tf | 426.91 | K | Joback Method |
| vc | 0.640 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 411.07 | J/mol×K | 672.75 | Joback Method |
| cpg | 462.02 | J/mol×K | 854.92 | Joback Method |
| cpg | 453.40 | J/mol×K | 818.48 | Joback Method |
| cpg | 444.00 | J/mol×K | 782.05 | Joback Method |
| cpg | 433.81 | J/mol×K | 745.62 | Joback Method |
| cpg | 422.83 | J/mol×K | 709.18 | Joback Method |
| cpg | 469.86 | J/mol×K | 891.35 | Joback Method |
| dvisc | 0.0001548 | Pa×s | 672.75 | Joback Method |
| dvisc | 0.0001921 | Pa×s | 631.78 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002455 | Pa×s | 590.80 | Joback Method |
| dvisc | 0.0003255 | Pa×s | 549.83 | Joback Method |
| dvisc | 0.0004516 | Pa×s | 508.86 | Joback Method |
| dvisc | 0.0006636 | Pa×s | 467.88 | Joback Method |
| dvisc | 0.0010498 | Pa×s | 426.91 | 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=U308343&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |