# Acetic acid, (5-chloro-2-nitrophenyl)methyl ester

**Inchi:** InChI=1S/C9H8ClNO4/c1-6(12)15-5-7-4-8(10)2-3-9(7)11(13)14/h2-4H,5H2,1H3
**InchiKey:** CXXIIBNSKGJPIM-UHFFFAOYSA-N
**Formula:** C9H8ClNO4
**SMILES:** CC(=O)OCc1cc(Cl)ccc1[N+](=O)[O-]
**Mol. weight [g/mol]:** 229.62

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -92.25 | kJ/mol | Joback Method |
| hf | -286.80 | kJ/mol | Joback Method |
| hfus | 30.67 | kJ/mol | Joback Method |
| hvap | 69.36 | kJ/mol | Joback Method |
| log10ws | -3.39 | | Crippen Method |
| logp | 2.311 | | Crippen Method |
| mcvol | 151.010 | ml/mol | McGowan Method |
| pc | 3228.31 | kPa | Joback Method |
| rinpol | 1696.00 | | NIST Webbook |
| rinpol | 1696.00 | | NIST Webbook |
| tb | 707.52 | K | Joback Method |
| tc | 953.17 | K | Joback Method |
| tf | 488.34 | K | Joback Method |
| vc | 0.587 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 365.58 | J/mol×K | 707.52 | Joback Method |
| cpg | 375.84 | J/mol×K | 748.46 | Joback Method |
| cpg | 385.27 | J/mol×K | 789.40 | Joback Method |
| cpg | 393.87 | J/mol×K | 830.35 | Joback Method |
| cpg | 401.66 | J/mol×K | 871.29 | Joback Method |
| cpg | 408.66 | J/mol×K | 912.23 | Joback Method |
| cpg | 414.88 | J/mol×K | 953.17 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U368733&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |