# 3-Chloro-2,4-pentanedione

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|---|---|
| **Other names:** | 3-Chloroacetylacetone |
| | 2,4-Pentanedione, 3-chloro- |
| | 1-Acetyl-1-chloroacetone |
| | 3-chloropentane-2,4-dione |
| | 3-Chloro.2,4-pentanedione |
| **Inchi:** | InChI=1S/C5H7ClO2/c1-3(7)5(6)4(2)8/h5H,1-2H3 |
| **InchiKey:** | VLRGXXKFHVJQOL-UHFFFAOYSA-N |
| **Formula:** | C5H7ClO2 |
| **SMILES:** | CC(=O)C(Cl)C(C)=O |
| **Mol. weight [g/mol]:** | 134.56 |
| **CAS:** | 1694-29-7 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -280.99 | kJ/mol | Joback Method |
| hf | -392.71 | kJ/mol | Joback Method |
| hfus | 12.58 | kJ/mol | Joback Method |
| hvap | 44.21 | kJ/mol | Joback Method |
| log10ws | -0.74 | | Crippen Method |
| logp | 0.772 | | Crippen Method |
| mcvol | 96.690 | ml/mol | McGowan Method |
| pc | 3901.37 | kPa | Joback Method |
| tb | 458.53 | K | Joback Method |
| tc | 661.35 | K | Joback Method |
| tf | 260.89 | K | Joback Method |
| vc | 0.370 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 178.43 | J/mol×K | 458.53 | Joback Method |
| cpg | 186.50 | J/mol×K | 492.33 | Joback Method |
| cpg | 194.18 | J/mol×K | 526.14 | Joback Method |
| cpg | 201.45 | J/mol×K | 559.94 | Joback Method |

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|---|---|---|---|---|
| cpg | 208.34 | J/mol×K | 593.74 | Joback Method |
| cpg | 214.85 | J/mol×K | 627.55 | Joback Method |
| cpg | 220.99 | J/mol×K | 661.35 | Joback Method |
| dvisc | 0.0046009 | Pa×s | 260.89 | Joback Method |
| dvisc | 0.0024329 | Pa×s | 293.83 | Joback Method |
| dvisc | 0.0014629 | Pa×s | 326.77 | Joback Method |
| dvisc | 0.0009655 | Pa×s | 359.71 | Joback Method |
| dvisc | 0.0006832 | Pa×s | 392.65 | Joback Method |
| dvisc | 0.0005101 | Pa×s | 425.59 | Joback Method |
| dvisc | 0.0003971 | Pa×s | 458.53 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 323.70 | K | 2.40 | NIST Webbook |

# Sources

**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
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C1694297&Units=SI

# 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

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