# p-(Chlorophenyl)acetone

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|---|---|
| **Other names:** | 2-Propanone, 1-(4-chlorophenyl)- |
| | 2-Propanone,p-chlorophenyl- |
| | 1-(p-Chlorophenyl)acetone |
| | NSC 22985 |
| | Methyl p-chlorobenzyl ketone |
| **Inchi:** | InChI=1S/C9H9ClO/c1-7(11)6-8-2-4-9(10)5-3-8/h2-5H,6H2,1H3 |
| **InchiKey:** | WEJRYKSUUFKMBC-UHFFFAOYSA-N |
| **Formula:** | C9H9ClO |
| **SMILES:** | CC(=O)Cc1ccc(Cl)cc1 |
| **Mol. weight [g/mol]:** | 168.62 |
| **CAS:** | 5586-88-9 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -13.17 | kJ/mol | Joback Method |
| hf | -132.35 | kJ/mol | Joback Method |
| hfus | 18.51 | kJ/mol | Joback Method |
| hvap | 49.70 | kJ/mol | Joback Method |
| log10ws | -2.66 | | Crippen Method |
| logp | 2.471 | | Crippen Method |
| mcvol | 127.720 | ml/mol | McGowan Method |
| pc | 3302.95 | kPa | Joback Method |
| tb | 528.28 | K | Joback Method |
| tc | 753.10 | K | Joback Method |
| tf | 309.98 | K | Joback Method |
| vc | 0.486 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 258.49 | J/mol×K | 528.28 | Joback Method |
| cpg | 310.02 | J/mol×K | 715.63 | Joback Method |
| cpg | 301.10 | J/mol×K | 678.16 | Joback Method |
| cpg | 291.51 | J/mol×K | 640.69 | Joback Method |

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|---|---|---|---|---|
| cpg | 281.24 | J/mol×K | 603.22 | Joback Method |
| cpg | 270.24 | J/mol×K | 565.75 | Joback Method |
| cpg | 318.31 | J/mol×K | 753.10 | Joback Method |
| dvisc | 0.0002769 | Pa×s | 528.28 | Joback Method |
| dvisc | 0.0003443 | Pa×s | 491.90 | Joback Method |
| dvisc | 0.0004434 | Pa×s | 455.51 | Joback Method |
| dvisc | 0.0005966 | Pa×s | 419.13 | Joback Method |
| dvisc | 0.0008494 | Pa×s | 382.75 | Joback Method |
| dvisc | 0.0013025 | Pa×s | 346.36 | Joback Method |
| dvisc | 0.0022080 | Pa×s | 309.98 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C5586889&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

**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
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume