# 4-Chlorophenyl benzoate

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|---|---|
| **Other names:** | Benzoic acid, 4-chlorophenyl ester |
| | p-Chlorophenol benzoate |
| | p-Chlorophenyl benzoate |
| | Benzoic acid, p-chlorophenyl ester |
| **Inchi:** | InChI=1S/C13H9ClO2/c14-11-6-8-12(9-7-11)16-13(15)10-4-2-1-3-5-10/h1-9H |
| **InchiKey:** | JKSIXXOEIXUYFW-UHFFFAOYSA-N |
| **Formula:** | C13H9ClO2 |
| **SMILES:** | O=C(Oc1ccc(Cl)cc1)c1ccccc1 |
| **Mol. weight [g/mol]:** | 232.66 |
| **CAS:** | 2005-08-5 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 27.92 | kJ/mol | Joback Method |
| hf | -110.60 | kJ/mol | Joback Method |
| hfus | 24.10 | kJ/mol | Joback Method |
| hvap | 63.29 | kJ/mol | Joback Method |
| log10ws | -4.24 | | Crippen Method |
| logp | 3.559 | | Crippen Method |
| mcvol | 166.190 | ml/mol | McGowan Method |
| pc | 3052.41 | kPa | Joback Method |
| rinpol | 1904.00 | | NIST Webbook |
| rinpol | 1904.00 | | NIST Webbook |
| tb | 668.90 | K | Joback Method |
| tc | 920.71 | K | Joback Method |
| tf | 403.71 | K | Joback Method |
| vc | 0.621 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 389.69 | J/mol×K | 668.90 | Joback Method |
| cpg | 444.92 | J/mol×K | 878.74 | Joback Method |
| cpg | 435.96 | J/mol×K | 836.77 | Joback Method |

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|---|---|---|---|---|
| cpg | 426.00 | J/mol×K | 794.80 | Joback Method |
| cpg | 415.01 | J/mol×K | 752.84 | Joback Method |
| cpg | 402.92 | J/mol×K | 710.87 | Joback Method |
| cpg | 452.94 | J/mol×K | 920.71 | Joback Method |
| dvisc | 0.0001568 | Pa×s | 668.90 | Joback Method |
| dvisc | 0.0001956 | Pa×s | 624.70 | Joback Method |
| dvisc | 0.0002524 | Pa×s | 580.50 | Joback Method |
| dvisc | 0.0003395 | Pa×s | 536.31 | Joback Method |
| dvisc | 0.0004818 | Pa×s | 492.11 | Joback Method |
| dvisc | 0.0007326 | Pa×s | 447.91 | Joback Method |
| dvisc | 0.0012209 | Pa×s | 403.71 | Joback Method |

# 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=C2005085&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
**pc:** Critical Pressure
**rinpol:** Non-polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume