# Benzoyl chloride, 3-chloro-

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|---|---|
| **Other names:** | 3-Chlorobenzoyl chloride |
| | Benzoyl chloride, m-chloro- |
| | m-Chlorobenzoyl chloride |
| **Inchi:** | InChI=1S/C7H4Cl2O/c8-6-3-1-2-5(4-6)7(9)10/h1-4H |
| **InchiKey:** | WHIHIKVIWVIIER-UHFFFAOYSA-N |
| **Formula:** | C7H4Cl2O |
| **SMILES:** | O=C(Cl)c1cccc(Cl)c1 |
| **Mol. weight [g/mol]:** | 175.01 |
| **CAS:** | 618-46-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -41.94 | kJ/mol | Joback Method |
| hf | -106.81 | kJ/mol | Joback Method |
| hfl | -190.00 ± 1.60 | kJ/mol | NIST Webbook |
| hfus | 17.53 | kJ/mol | Joback Method |
| hvap | 49.63 | kJ/mol | Joback Method |
| log10ws | -3.05 | | Crippen Method |
| logp | 2.719 | | Crippen Method |
| mcvol | 111.780 | ml/mol | McGowan Method |
| pc | 3980.54 | kPa | Joback Method |
| rinpol | 1246.60 | | NIST Webbook |
| rinpol | 1246.60 | | NIST Webbook |
| tb | 498.20 | K | NIST Webbook |
| tc | 758.29 | K | Joback Method |
| tf | 317.36 | K | Joback Method |
| vc | 0.423 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 239.57 | J/mol×K | 758.29 | Joback Method |
| cpg | 233.90 | J/mol×K | 718.56 | Joback Method |
| cpg | 227.70 | J/mol×K | 678.84 | Joback Method |

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|---|---|---|---|---|
| cpg | 220.95 | J/mol×K | 639.12 | Joback Method |
| cpg | 213.61 | J/mol×K | 599.40 | Joback Method |
| cpg | 205.65 | J/mol×K | 559.67 | Joback Method |
| cpg | 197.03 | J/mol×K | 519.95 | Joback Method |
| dvisc | 0.0021445 | Pa×s | 317.36 | Joback Method |
| dvisc | 0.0003235 | Pa×s | 519.95 | Joback Method |
| dvisc | 0.0003974 | Pa×s | 486.19 | Joback Method |
| dvisc | 0.0005035 | Pa×s | 452.42 | Joback Method |
| dvisc | 0.0006626 | Pa×s | 418.66 | Joback Method |
| dvisc | 0.0009150 | Pa×s | 384.89 | Joback Method |
| dvisc | 0.0013446 | Pa×s | 351.12 | Joback Method |
| hvapt | 49.40 | kJ/mol | 379.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.36924e+01 |
| Coeff. B | -4.29827e+03 |
| Coeff. C | -4.80940e+01 |
| Temperature range (K), min. | 368.75 |
| Temperature range (K), max. | 560.96 |

# Sources

**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=C618462&Units=SI

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

**cpg:** Ideal gas heat capacity

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|---|---|
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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