# Phenol, 3-chloro-

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|---|---|
| **Other names:** | 3-Chlorophenol |
| | 3-Hydroxychlorobenzene |
| | NSC 59700 |
| | Phenol, m-chloro- |
| | m-Chlorophenic acid |
| | m-Chlorophenol |
| | meta-Chlorophenol |
| **Inchi:** | InChI=1S/C6H5ClO/c7-5-2-1-3-6(8)4-5/h1-4,8H |
| **InchiKey:** | HORNXRXVQWOLPJ-UHFFFAOYSA-N |
| **Formula:** | C6H5ClO |
| **SMILES:** | Oc1cccc(Cl)c1 |
| **Mol. weight [g/mol]:** | 128.56 |
| **CAS:** | 108-43-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -2910.00 ± 8.40 | kJ/mol | NIST Webbook |
| chs | -2890.00 ± 8.00 | kJ/mol | NIST Webbook |
| gf | -54.50 | kJ/mol | Joback Method |
| hf | -123.69 | kJ/mol | Joback Method |
| hfus | 15.32 | kJ/mol | Joback Method |
| hsub | 76.90 ± 0.30 | kJ/mol | NIST Webbook |
| hvap | 63.50 ± 0.30 | kJ/mol | NIST Webbook |
| ie | 8.65 ± 0.00 | eV | NIST Webbook |
| ie | 8.68 ± 0.00 | eV | NIST Webbook |
| ie | 8.65 ± 0.03 | eV | NIST Webbook |
| ie | 8.65 ± 0.00 | eV | NIST Webbook |
| log10ws | -0.70 | | Estimated Solubility Method |
| log10ws | -0.70 | | Aqueous Solubility Prediction Method |
| logp | 2.046 | | Crippen Method |
| mcvol | 89.750 | ml/mol | McGowan Method |
| pc | 5478.85 | kPa | Joback Method |
| rinpol | 1170.00 | | NIST Webbook |
| rinpol | 1167.00 | | NIST Webbook |
| rinpol | 1198.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1165.00 | | NIST Webbook |
| rinpol | 1169.00 | | NIST Webbook |
| rinpol | 1159.00 | | NIST Webbook |
| rinpol | 1200.00 | | NIST Webbook |
| rinpol | 1203.00 | | NIST Webbook |
| rinpol | 1194.00 | | NIST Webbook |
| rinpol | 1173.00 | | NIST Webbook |
| rinpol | 1171.00 | | NIST Webbook |
| rinpol | 1194.00 | | NIST Webbook |
| rinpol | 1189.00 | | NIST Webbook |
| rinpol | 1161.00 | | NIST Webbook |
| rinpol | 1157.00 | | NIST Webbook |
| rinpol | 1159.00 | | NIST Webbook |
| rinpol | 1194.00 | | NIST Webbook |
| rinpol | 1157.00 | | NIST Webbook |
| rinpol | 1203.30 | | NIST Webbook |
| rinpol | 1207.00 | | NIST Webbook |
| ripol | 2345.00 | | NIST Webbook |
| ripol | 2371.00 | | NIST Webbook |
| ripol | 2371.00 | | NIST Webbook |
| ripol | 2371.00 | | NIST Webbook |
| ripol | 2380.00 | | NIST Webbook |
| ripol | 2364.00 | | NIST Webbook |
| ripol | 2333.00 | | NIST Webbook |
| ripol | 2350.00 | | NIST Webbook |
| ripol | 2345.00 | | NIST Webbook |
| ripol | 2378.00 | | NIST Webbook |
| tb | 487.20 | K | NIST Webbook |
| tc | 721.38 | K | Joback Method |
| tf | 305.80 ± 0.20 | K | NIST Webbook |
| tf | 305.50 | K | Solid liquid equilibria of mixtures containing tert-butanol, m-chlorophenol, and p-chlorophenol and development of adductive crystallization processes |
| tf | 306.08 | K | Aqueous Solubility Prediction Method |
| vc | 0.279 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
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| cpg | 167.36 | J/mol×K | 481.41 | Joback Method |
| cpg | 183.82 | J/mol×K | 561.40 | Joback Method |
| cpg | 190.92 | J/mol×K | 601.39 | Joback Method |
| cpg | 197.38 | J/mol×K | 641.39 | Joback Method |
| cpg | 203.28 | J/mol×K | 681.38 | Joback Method |
| cpg | 208.73 | J/mol×K | 721.38 | Joback Method |
| cpg | 176.00 | J/mol×K | 521.40 | Joback Method |
| dvisc | 0.0009700 | Pa×s | 377.43 | Joback Method |
| dvisc | 0.0005253 | Pa×s | 403.42 | Joback Method |
| dvisc | 0.0044385 | Pa×s | 325.44 | Joback Method |
| dvisc | 0.0003064 | Pa×s | 429.42 | Joback Method |
| dvisc | 0.0001900 | Pa×s | 455.41 | Joback Method |
| dvisc | 0.0001241 | Pa×s | 481.41 | Joback Method |
| dvisc | 0.0019615 | Pa×s | 351.44 | Joback Method |
| hfust | 14.90 | kJ/mol | 305.80 | NIST Webbook |
| hfust | 14.91 | kJ/mol | 305.80 | NIST Webbook |
| hfust | 14.91 | kJ/mol | 305.80 | NIST Webbook |
| hsubt | 53.00 ± 1.00 | kJ/mol | 301.00 | NIST Webbook |
| hvapt | 61.90 | kJ/mol | 321.50 | NIST Webbook |
| hvapt | 53.10 | kJ/mol | 402.00 | NIST Webbook |
| psub | 2.62e-03 | kPa | 285.20 | Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions |
| psub | 9.99e-03 | kPa | 297.30 | Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions |
| psub | 7.21e-03 | kPa | 294.30 | Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions |

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|---|---|---|---|---|---|
| psub | 5.09e-03 | kPa | 291.30 | Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions | |
| psub | 3.66e-03 | kPa | 288.30 | Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions | |
| psub | 0.01 | kPa | 300.30 | Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions | |
| psub | 2.12e-03 | kPa | 283.20 | Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions | |
| psub | 1.49e-03 | kPa | 280.30 | Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions | |

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|---|---|---|---|---|
| psub | 1.15e-03 | kPa | 278.30 | Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions |
| psub | 9.50e-04 | kPa | 276.60 | Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions |
| psub | 8.20e-04 | kPa | 275.30 | Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions |
| psub | 0.02 | kPa | 302.20 | Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions |
| psub | 0.02 | kPa | 306.00 | Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions |
| sfust | 48.74 | J/mol×K | 305.80 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 2.34612e+01 |
| Coeff. B | -7.98338e+03 |
| Coeff. C | -1.48550e+01 |
| Temperature range (K), min. | 359.36 |
| Temperature range (K), max. | 454.72 |

# Sources

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|---|---|
| **Solid liquid equilibria of mixtures containing tert-butanol, m-cresol, and p-chlorophenol** | https://www.doi.org/10.1016/j.fluid.2005.08.021 |
| **Thermochemistry of Chlorobenzenes and Chlorophenols: Analysis of Vapor Pressures and Enthalpies of Phase Transitions:** | https://www.doi.org/10.1021/je060429r |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C108430&Units=SI |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **Investigating the solubility of chlorophenols in hydrophobic ionic liquids:** | https://www.doi.org/10.1016/j.jct.2019.03.026 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **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

| | |
|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **chs:** | Standard solid enthalpy of combustion |
| **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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hsub:** | Enthalpy of sublimation at standard conditions |
| **hsubt:** | Enthalpy of sublimation at a given temperature |

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|---|---|
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **psub:** | Sublimation pressure |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **sfust:** | Entropy of fusion at a given temperature |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |