# Benzene, 1,3,5-trichloro-

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|---|---|
| **Other names:** | 1,3,5-Trichlorobenzene |
| | SYM-TRICHLOROBENZENE |
| | UN 2321 |
| | s-Trichlorobenzene |
| **Inchi:** | InChI=1S/C6H3Cl3/c7-4-1-5(8)3-6(9)2-4/h1-3H |
| **InchiKey:** | XKEFYDZQGKAQCN-UHFFFAOYSA-N |
| **Formula:** | C6H3Cl3 |
| **SMILES:** | Clc1cc(Cl)cc(Cl)c1 |
| **Mol. weight [g/mol]:** | 181.45 |
| **CAS:** | 108-70-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -2785.40 ± 1.30 | kJ/mol | NIST Webbook |
| chs | -2781.96 ± 0.51 | kJ/mol | NIST Webbook |
| ea | 0.34 | eV | NIST Webbook |
| gf | 57.00 | kJ/mol | Joback Method |
| hf | -2.60 ± 1.40 | kJ/mol | NIST Webbook |
| hf | -13.36 | kJ/mol | NIST Webbook |
| hfs | -75.30 ± 1.30 | kJ/mol | NIST Webbook |
| hfus | 17.56 | kJ/mol | Low-Temperature Heat Capacities and Derived Thermodynamic Functions of 1,4 Dichlorobenzene, 1,4 Dibromobenzene, 1,3,5 Trichlorobenzene, and 1,3,5 Tribromobenzene |
| hsub | 72.70 ± 0.50 | kJ/mol | NIST Webbook |
| hsub | 54.02 | kJ/mol | NIST Webbook |
| hsub | 72.70 ± 0.50 | kJ/mol | NIST Webbook |
| hvap | 59.00 | kJ/mol | NIST Webbook |
| ie | 9.34 ± 0.02 | eV | NIST Webbook |
| ie | 9.50 ± 0.15 | eV | NIST Webbook |
| ie | 9.32 ± 0.03 | eV | NIST Webbook |
| ie | 9.20 | eV | NIST Webbook |
| ie | 9.30 | eV | NIST Webbook |
| ie | 9.30 ± 0.06 | eV | NIST Webbook |
| ie | 9.36 | eV | NIST Webbook |

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|---|---|---|---|
| log10ws | -4.54 | | Aqueous Solubility Prediction Method |
| log10ws | -4.48 | | Estimated Solubility Method |
| log10ws | -4.44 | | Aqueous and cosolvent solubility data for drug-like organic compounds |
| logp | 3.647 | | Crippen Method |
| mcvol | 108.360 | ml/mol | McGowan Method |
| pc | 3886.79 | kPa | Joback Method |
| rinpol | 1113.00 | | NIST Webbook |
| rinpol | 1122.94 | | NIST Webbook |
| rinpol | 1106.00 | | NIST Webbook |
| rinpol | 1112.00 | | NIST Webbook |
| rinpol | 1151.00 | | NIST Webbook |
| rinpol | 1131.00 | | NIST Webbook |
| rinpol | 1150.00 | | NIST Webbook |
| rinpol | 190.00 | | NIST Webbook |
| rinpol | 190.00 | | NIST Webbook |
| rinpol | 1145.00 | | NIST Webbook |
| rinpol | 1158.00 | | NIST Webbook |
| rinpol | 1150.00 | | NIST Webbook |
| rinpol | 1162.50 | | NIST Webbook |
| rinpol | 1153.70 | | NIST Webbook |
| rinpol | 1165.10 | | NIST Webbook |
| rinpol | 1146.29 | | NIST Webbook |
| rinpol | 1122.94 | | NIST Webbook |
| rinpol | 1133.72 | | NIST Webbook |
| rinpol | 1091.00 | | NIST Webbook |
| rinpol | 1131.00 | | NIST Webbook |
| rinpol | 1150.00 | | NIST Webbook |
| rinpol | 1131.00 | | NIST Webbook |
| rinpol | 1144.00 | | NIST Webbook |
| rinpol | 1150.00 | | NIST Webbook |
| rinpol | 1117.64 | | NIST Webbook |
| rinpol | 1122.48 | | NIST Webbook |
| rinpol | 1127.13 | | NIST Webbook |
| rinpol | 1128.00 | | NIST Webbook |
| rinpol | 1123.00 | | NIST Webbook |
| rinpol | 1115.00 | | NIST Webbook |
| rinpol | 1109.00 | | NIST Webbook |
| rinpol | 1112.00 | | NIST Webbook |
| rinpol | 1146.00 | | NIST Webbook |
| rinpol | 1084.00 | | NIST Webbook |
| rinpol | 1095.00 | | NIST Webbook |
| rinpol | 1096.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1100.00 | | NIST Webbook |
| rinpol | 1131.00 | | NIST Webbook |
| ripol | 1515.00 | | NIST Webbook |
| ripol | 1550.00 | | NIST Webbook |
| ripol | 1589.50 | | NIST Webbook |
| ripol | 1545.00 | | NIST Webbook |
| ripol | 1550.00 | | NIST Webbook |
| ripol | 1517.60 | | NIST Webbook |
| ripol | 1529.51 | | NIST Webbook |
| ripol | 1517.48 | | NIST Webbook |
| ripol | 1517.29 | | NIST Webbook |
| ripol | 1590.00 | | NIST Webbook |
| ripol | 1545.00 | | NIST Webbook |
| ripol | 1515.00 | | NIST Webbook |
| ripol | 1569.30 | | NIST Webbook |
| tb | 481.20 | K | NIST Webbook |
| tc | 725.08 | K | Joback Method |
| tf | 337.30 | K | Aqueous Solubility Prediction Method |
| tf | 336.20 ± 0.50 | K | NIST Webbook |
| tf | 336.70 ± 0.10 | K | NIST Webbook |
| tf | 336.30 ± 0.20 | K | NIST Webbook |
| tf | 334.45 ± 0.20 | K | NIST Webbook |
| vc | 0.410 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 182.83 | J/mol×K | 565.43 | Joback Method |
| cpg | 204.95 | J/mol×K | 725.08 | Joback Method |
| cpg | 200.07 | J/mol×K | 685.17 | Joback Method |
| cpg | 194.78 | J/mol×K | 645.26 | Joback Method |
| cpg | 189.04 | J/mol×K | 605.34 | Joback Method |
| cpg | 168.92 | J/mol×K | 485.61 | Joback Method |
| cpg | 176.13 | J/mol×K | 525.52 | Joback Method |
| dvisc | 0.0004556 | Pa×s | 423.27 | Joback Method |
| dvisc | 0.0003679 | Pa×s | 454.44 | Joback Method |
| dvisc | 0.0003053 | Pa×s | 485.61 | Joback Method |
| dvisc | 0.0011033 | Pa×s | 329.77 | Joback Method |
| dvisc | 0.0007808 | Pa×s | 360.94 | Joback Method |
| dvisc | 0.0016757 | Pa×s | 298.60 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0005838 | Pa×s | 392.11 | Joback Method |
| hfust | 17.56 | kJ/mol | 335.90 | NIST Webbook |
| hfust | 18.20 | kJ/mol | 336.70 | NIST Webbook |
| hfust | 18.20 | kJ/mol | 336.70 | NIST Webbook |
| hsubt | 56.50 | kJ/mol | 291.50 | NIST Webbook |
| hvapt | 48.80 | kJ/mol | 409.00 | NIST Webbook |
| hvapt | 51.70 | kJ/mol | 337.00 | NIST Webbook |
| hvapt | 50.30 ± 0.10 | kJ/mol | 376.50 | NIST Webbook |
| rhos | 1446.70 | kg/m3 | 298.15 | Determination and thermodynamic modeling of solid-liquid phase equilibrium for 3,5-dichloroaniline in pure solvents and ternary 3,5-dichloroaniline + 1,3,5-trichlorobenzene + toluene system |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.37196e+01 |
| Coeff. B | -3.69674e+03 |
| Coeff. C | -7.50210e+01 |
| Temperature range (K), min. | 336.65 |
| Temperature range (K), max. | 514.68 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 6.93529e+01 |
| Coeff. B | -8.25027e+03 |
| Coeff. C | -7.86946e+00 |
| Coeff. D | 4.33587e-06 |
| Temperature range (K), min. | 336.15 |
| Temperature range (K), max. | 482.15 |

# Sources

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|---|---|
| **Solubility and Dissolution Thermodynamics for 1,3,5-Trichlorobenzene in Organic Solvents:** | https://www.doi.org/10.1021/acs.jced.5b00607 |
| **Low-Temperature Heat Capacities and Derived Thermodynamic Functions of 1,4 Dichlorobenzene, 1,4 Dibromobenzene, 1,3,5 Trichlorobenzene, and 1,3,5 Tribromobenzene:** | https://www.doi.org/10.1021/je049762q |
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol1672.mol |
| **Determination and thermodynamic modeling of solid-liquid phase equilibria of 3,5-dichloroaniline in pure solvents and ternary 3,5-dichloroaniline + 1,2,3-trichlorobenzene + toluene system:** | https://www.doi.org/10.1016/j.jct.2016.03.007 |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1672 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C108703&Units=SI |
| **Aqueous and cosolvent solubility data for drug-like organic compounds:** | https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/ |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **ea:** | Electron affinity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase 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 |
| **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 |
| **pvap:** | Vapor pressure |
| **rhos:** | Solid Density |
| **rinpol:** | Non-polar retention indices |

| | |
|---|---|
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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