# Benzene, 1,2,4-trichloro-

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|---|---|
| **Other names:** | 1,2,4-Trichlorobenzene |
| | 1,2,4-Trichlorobenzol |
| | 1,2,5-TRICHLOROBENZENE |
| | 1,3,4-Trichlorobenzene |
| | AS-TRICHLOROBENZENE |
| | Hipochem GM |
| | Hostetex L-PEC |
| | NSC 406697 |
| | Trojchlorobenzen |
| | unsym-Trichlorobenzene |
| **Inchi:** | InChI=1S/C6H3Cl3/c7-4-1-2-5(8)6(9)3-4/h1-3H |
| **InchiKey:** | PBKONEOXTCPAFI-UHFFFAOYSA-N |
| **Formula:** | C6H3Cl3 |
| **SMILES:** | Clc1ccc(Cl)c(Cl)c1 |
| **Mol. weight [g/mol]:** | 181.45 |
| **CAS:** | 120-82-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -2797.98 ± 0.44 | kJ/mol | NIST Webbook |
| chl | -2810.50 ± 1.50 | kJ/mol | NIST Webbook |
| gf | 57.00 | kJ/mol | Joback Method |
| hf | 4.90 ± 1.60 | kJ/mol | NIST Webbook |
| hf | -8.05 | kJ/mol | NIST Webbook |
| hfl | -50.20 ± 1.50 | kJ/mol | NIST Webbook |
| hfus | 17.15 | kJ/mol | Joback Method |
| hvap | 55.50 ± 0.10 | kJ/mol | NIST Webbook |
| hvap | 55.10 ± 0.50 | kJ/mol | NIST Webbook |
| hvap | 54.68 | kJ/mol | NIST Webbook |
| hvap | 57.60 | kJ/mol | NIST Webbook |
| ie | 9.04 ± 0.03 | eV | NIST Webbook |
| log10ws | -3.60 | | Aqueous Solubility Prediction Method |
| log10ws | -3.59 | | Estimated Solubility Method |
| logp | 3.647 | | Crippen Method |
| mcvol | 108.360 | ml/mol | McGowan Method |

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|---|---|---|---|
| nfpaf | %!d(float64=1) | | KDB |
| nfpah | %!d(float64=2) | | KDB |
| nfpas | %!d(float64=3) | | KDB |
| pc | 3886.79 | kPa | Joback Method |
| rinpol | 1193.06 | | NIST Webbook |
| rinpol | 1189.56 | | NIST Webbook |
| rinpol | 1164.56 | | NIST Webbook |
| rinpol | 1176.18 | | NIST Webbook |
| rinpol | 1177.00 | | NIST Webbook |
| rinpol | 1193.00 | | NIST Webbook |
| rinpol | 1177.00 | | NIST Webbook |
| rinpol | 1183.00 | | NIST Webbook |
| rinpol | 1193.00 | | NIST Webbook |
| rinpol | 1186.00 | | NIST Webbook |
| rinpol | 1177.00 | | NIST Webbook |
| rinpol | 1161.00 | | NIST Webbook |
| rinpol | 1166.00 | | NIST Webbook |
| rinpol | 1192.67 | | NIST Webbook |
| rinpol | 1199.70 | | NIST Webbook |
| rinpol | 1196.72 | | NIST Webbook |
| rinpol | 1196.78 | | NIST Webbook |
| rinpol | 1141.60 | | NIST Webbook |
| rinpol | 1158.50 | | NIST Webbook |
| rinpol | 1160.14 | | NIST Webbook |
| rinpol | 1166.23 | | NIST Webbook |
| rinpol | 1171.69 | | NIST Webbook |
| rinpol | 1168.00 | | NIST Webbook |
| rinpol | 1189.60 | | NIST Webbook |
| rinpol | 1157.00 | | NIST Webbook |
| rinpol | 1150.00 | | NIST Webbook |
| rinpol | 1152.00 | | NIST Webbook |
| rinpol | 1172.00 | | NIST Webbook |
| rinpol | 1160.00 | | NIST Webbook |
| rinpol | 1198.00 | | NIST Webbook |
| rinpol | 1142.00 | | NIST Webbook |
| rinpol | 1144.00 | | NIST Webbook |
| rinpol | 1145.00 | | NIST Webbook |
| rinpol | 1149.00 | | NIST Webbook |
| rinpol | 1170.00 | | NIST Webbook |
| rinpol | 1177.00 | | NIST Webbook |
| rinpol | 1174.00 | | NIST Webbook |
| rinpol | 1158.00 | | NIST Webbook |
| rinpol | 1145.00 | | NIST Webbook |
| rinpol | 1193.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1150.00 | | NIST Webbook |
| rinpol | 1154.00 | | NIST Webbook |
| rinpol | 199.00 | | NIST Webbook |
| rinpol | 198.20 | | NIST Webbook |
| rinpol | 1142.00 | | NIST Webbook |
| rinpol | 1193.67 | | NIST Webbook |
| rinpol | 1193.56 | | NIST Webbook |
| rinpol | 1150.00 | | NIST Webbook |
| rinpol | 1211.10 | | NIST Webbook |
| rinpol | 1162.00 | | NIST Webbook |
| ripol | 1630.00 | | NIST Webbook |
| ripol | 1671.43 | | NIST Webbook |
| ripol | 1643.59 | | NIST Webbook |
| ripol | 1658.54 | | NIST Webbook |
| ripol | 1665.50 | | NIST Webbook |
| ripol | 1659.76 | | NIST Webbook |
| ripol | 1688.60 | | NIST Webbook |
| ripol | 1698.00 | | NIST Webbook |
| ripol | 1653.00 | | NIST Webbook |
| ripol | 1630.00 | | NIST Webbook |
| tb | 486.70 | K | NIST Webbook |
| tc | 725.08 | K | Joback Method |
| tf | 282.20 ± 4.00 | K | NIST Webbook |
| tf | 289.70 ± 3.00 | K | NIST Webbook |
| tf | 290.10 ± 0.02 | 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 |

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|---|---|---|---|---|
| cpl | 204.61 | J/mol×K | 349.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 205.35 | J/mol×K | 353.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 194.60 | J/mol×K | 298.15 | NIST Webbook |
| cpl | 188.00 | J/mol×K | 297.95 | NIST Webbook |
| cpl | 194.90 | J/mol×K | 298.15 | NIST Webbook |
| cpl | 194.25 | J/mol×K | 293.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 194.57 | J/mol×K | 295.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 204.98 | J/mol×K | 351.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 195.23 | J/mol×K | 299.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 195.57 | J/mol×K | 301.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 195.92 | J/mol×K | 303.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |

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|---|---|---|---|---|
| cpl | 196.27 | J/mol×K | 305.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 196.63 | J/mol×K | 307.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 196.99 | J/mol×K | 309.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 197.35 | J/mol×K | 311.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 197.72 | J/mol×K | 313.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 198.09 | J/mol×K | 315.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 198.47 | J/mol×K | 317.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 198.85 | J/mol×K | 319.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 199.23 | J/mol×K | 321.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |

| | | | | |
|---|---|---|---|---|
| cpl | 199.61 | J/mol×K | 323.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 200.00 | J/mol×K | 325.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 200.38 | J/mol×K | 327.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 200.77 | J/mol×K | 329.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 201.16 | J/mol×K | 331.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 201.55 | J/mol×K | 333.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 201.93 | J/mol×K | 335.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 202.32 | J/mol×K | 337.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |

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|---|---|---|---|---|
| cpl | 202.71 | J/mol×K | 339.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 203.09 | J/mol×K | 341.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 203.47 | J/mol×K | 343.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 203.85 | J/mol×K | 345.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 204.23 | J/mol×K | 347.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 194.90 | J/mol×K | 297.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| dvisc | 0.0011033 | Pa×s | 329.77 | Joback Method |
| dvisc | 0.0003053 | Pa×s | 485.61 | Joback Method |
| dvisc | 0.0003679 | Pa×s | 454.44 | Joback Method |
| dvisc | 0.0005838 | Pa×s | 392.11 | Joback Method |
| dvisc | 0.0007808 | Pa×s | 360.94 | Joback Method |
| dvisc | 0.0016757 | Pa×s | 298.60 | Joback Method |
| dvisc | 0.0004556 | Pa×s | 423.27 | Joback Method |
| hsubt | 62.30 | kJ/mol | 288.50 | NIST Webbook |
| hvapt | 55.80 | kJ/mol | 290.00 | NIST Webbook |
| hvapt | 49.50 | kJ/mol | 440.50 | NIST Webbook |
| hvapt | 47.00 | kJ/mol | 288.50 | NIST Webbook |
| hvapt | 49.30 | kJ/mol | 398.50 | NIST Webbook |

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| rfi | 1.54300 | | 308.15 | Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 2-Octanol with Chlorobenzenes |
| rfi | 1.52200 | | 298.15 | Liquid-Liquid Equilibria for Mixtures of (Furfural + a Chlorinated Aromatic Compound + an Alkane) at T = 298.15 K |
| rfi | 1.54600 | | 303.15 | Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 2-Octanol with Chlorobenzenes |
| rfi | 1.54800 | | 298.15 | Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 2-Octanol with Chlorobenzenes |
| rhol | 1442.12 | kg/m3 | 303.15 | Effect of various substituents on benzene ring and their impact on volumetric, acoustic and transport properties of binary liquid mixtures with dimethylacetamide |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.49608e+01 |
| Coeff. B | -4.65563e+03 |

| | |
|---|---|
| Coeff. C | -3.65540e+01 |
| Temperature range (K), min. | 353.84 |
| Temperature range (K), max. | 519.04 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 3.43692e+01 |
| Coeff. B | -6.72270e+03 |
| Coeff. C | -2.58415e+00 |
| Coeff. D | 2.74692e-07 |
| Temperature range (K), min. | 290.15 |
| Temperature range (K), max. | 725.00 |

# Datasets

## Viscosity, Pa*s

| Pressure, kPa - Liquid | Temperature, K - Liquid | Viscosity, Pa*s - Liquid |
|---|---|---|
| 101.00 | 303.15 | 0.0016130 |

Reference *https://www.doi.org/10.1016/j.jct.2006.04.005*

# Sources

| | |
|---|---|
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1670 |
| **Volumetric, ultrasonic and viscometric studies of binary mixtures of dimethyl sulphoxide with chloro and nitro substituted aromatic hydrocarbons at T = 303.15 K:** | https://www.doi.org/10.1016/j.jct.2006.04.005 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C120821&Units=SI |
| **Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes:** | https://www.doi.org/10.1021/je600573w |
| **Determination of Henry's Law Constant Using Diffusion in Air and Water Boundary Layers:** | https://www.doi.org/10.1021/je300954s |
| **Effect of various substituents on benzene ring and their impact on Crippen Method:** | https://www.doi.org/10.1016/j.fluid.2015.03.048 |
| **Volumetric, acoustic and transport properties of binary liquid mixtures with dimethylacetamide:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **Liquid-Liquid Equilibria for Mixtures of (Furfural + a Chlorinated Aromatic Compound + an Alkane) at T = 298.15 K:** | https://www.doi.org/10.1021/je020107x |
| **Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:** | https://www.doi.org/10.1021/je3010535 |

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|---|---|
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol1670.mol |
| **Densities and ultrasonic studies for binary mixtures of tetrahydrofuran with chlorobenzenes, chlorotoluenes and nitrotoluenes at 298.15 K:** | https://www.doi.org/10.1016/j.fluid.2011.07.018 |
| **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 |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 2-Octanol with Chlorobenzenes:** | https://www.doi.org/10.1007/s10765-011-1087-7 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

| | |
|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase heat capacity |
| **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 |
| **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 |
| **nfpaf:** | NFPA Fire Rating |
| **nfpah:** | NFPA Health Rating |
| **nfpas:** | NFPA Safety Rating |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rfi:** | Refractive Index |
| **rhol:** | Liquid 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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