# Benzene, 1,4-dichloro-

**Other names:**

1,4-DICHLOROBENZENE
1,4-Dichloorbenzeen
1,4-Dichlor-benzol
1,4-Diclorobenzene
1,4-chlorobenzene
Benzene, p-dichloro-
Di-chloricide
Dichlorobenzene
Dichlorobenzene, p-
Dichlorobenzene, para
Dichlorocide
Evola
Globol
Kaydox
NCI-C54955
NSC 36935
P-DICHLOROBENZENE
PDB
Paracide
Paradi
Paradichlorbenzol
Paradichlorobenzol
Paradow
Paramoth
Paranuggets
Parazene
Persia-Perazol
Rcra waste number U070
Rcra waste number U071
Rcra waste number U072
SANTOCHLOR
UN 1592
p-Chlorophenyl chloride
p-Dichloorbenzeen
p-Dichlorbenzene
p-Dichlorbenzol
p-Dichlorobenzol
p-Diclorobenzene
para crystals
para-Dichlorobenzene

**Inchi:** InChI=1S/C6H4Cl2/c7-5-1-2-6(8)4-3-5/h1-4H
**InchiKey:** OCJBOOLMMGQPQU-UHFFFAOYSA-N
**Formula:** C6H4Cl2
**SMILES:** Clc1ccc(Cl)cc1
**Mol. weight [g/mol]:** 147.00
**CAS:** 106-46-7

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -2937.00 ± 4.00 | kJ/mol | NIST Webbook |
| chs | -2934.10 ± 1.00 | kJ/mol | NIST Webbook |
| chs | -2939.90 | kJ/mol | NIST Webbook |
| gf | 78.56 | kJ/mol | Joback Method |
| hf | 24.60 | kJ/mol | NIST Webbook |
| hfpi | 883.20 | kJ/mol | NIST Webbook |
| hfpiz | 895.80 | kJ/mol | NIST Webbook |
| hfs | -42.30 ± 1.00 | kJ/mol | NIST Webbook |
| hfus | 17.91 | 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 | 64.75 ± 0.15 | kJ/mol | NIST Webbook |
| hsub | 65.20 ± 2.00 | kJ/mol | NIST Webbook |
| hvap | 54.80 | kJ/mol | NIST Webbook |
| hvap | 47.80 | kJ/mol | NIST Webbook |
| ie | 8.95 | eV | NIST Webbook |
| ie | 8.97 ± 0.03 | eV | NIST Webbook |
| ie | 8.99 | eV | NIST Webbook |
| ie | 9.00 | eV | NIST Webbook |
| ie | 8.92 ± 0.02 | eV | NIST Webbook |
| ie | 8.94 | eV | NIST Webbook |
| ie | 8.98 ± 0.02 | eV | NIST Webbook |
| ie | 8.89 ± 0.01 | eV | NIST Webbook |
| ie | 8.94 ± 0.01 | eV | NIST Webbook |
| ie | 8.92 ± 0.03 | eV | NIST Webbook |
| ie | 8.95 | eV | NIST Webbook |
| log10ws | -3.29 | | Aqueous Solubility Prediction Method |

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|---|---|---|---|
| log10ws | -3.27 | | Estimated Solubility Method |
| logp | 2.993 | | Crippen Method |
| mcvol | 96.120 | ml/mol | McGowan Method |
| nfpaf | %!d(float64=2) | | KDB |
| nfpah | %!d(float64=2) | | KDB |
| pc | 4151.61 | kPa | Joback Method |
| rinpol | 985.00 | | NIST Webbook |
| rinpol | 1047.00 | | NIST Webbook |
| rinpol | 1029.00 | | NIST Webbook |
| rinpol | 988.00 | | NIST Webbook |
| rinpol | 986.00 | | NIST Webbook |
| rinpol | 987.00 | | NIST Webbook |
| rinpol | 1000.00 | | NIST Webbook |
| rinpol | 985.00 | | NIST Webbook |
| rinpol | 1050.00 | | NIST Webbook |
| rinpol | 988.00 | | NIST Webbook |
| rinpol | 1009.00 | | NIST Webbook |
| rinpol | 989.00 | | NIST Webbook |
| rinpol | 970.00 | | NIST Webbook |
| rinpol | 1057.00 | | NIST Webbook |
| rinpol | 1016.00 | | NIST Webbook |
| rinpol | 1014.00 | | NIST Webbook |
| rinpol | 1007.00 | | NIST Webbook |
| rinpol | 1024.00 | | NIST Webbook |
| rinpol | 995.00 | | NIST Webbook |
| rinpol | 994.00 | | NIST Webbook |
| rinpol | 1023.00 | | NIST Webbook |
| rinpol | 163.00 | | NIST Webbook |
| rinpol | 1015.00 | | NIST Webbook |
| rinpol | 162.00 | | NIST Webbook |
| rinpol | 163.15 | | NIST Webbook |
| rinpol | 164.81 | | NIST Webbook |
| rinpol | 1013.00 | | NIST Webbook |
| rinpol | 974.00 | | NIST Webbook |
| rinpol | 1023.15 | | NIST Webbook |
| rinpol | 1023.18 | | NIST Webbook |
| rinpol | 1032.51 | | NIST Webbook |
| rinpol | 1032.76 | | NIST Webbook |
| rinpol | 1016.00 | | NIST Webbook |
| rinpol | 1037.40 | | NIST Webbook |
| rinpol | 1037.40 | | NIST Webbook |
| rinpol | 974.00 | | NIST Webbook |
| rinpol | 1012.00 | | NIST Webbook |
| rinpol | 993.00 | | NIST Webbook |

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|---|---|---|
| rinpol | 970.00 | NIST Webbook |
| rinpol | 1016.00 | NIST Webbook |
| rinpol | 970.00 | NIST Webbook |
| rinpol | 1015.00 | NIST Webbook |
| rinpol | 1016.00 | NIST Webbook |
| rinpol | 1016.00 | NIST Webbook |
| rinpol | 1000.00 | NIST Webbook |
| rinpol | 1021.24 | NIST Webbook |
| rinpol | 1021.56 | NIST Webbook |
| rinpol | 1024.00 | NIST Webbook |
| rinpol | 1025.03 | NIST Webbook |
| rinpol | 1014.90 | NIST Webbook |
| rinpol | 991.21 | NIST Webbook |
| rinpol | 990.60 | NIST Webbook |
| rinpol | 989.50 | NIST Webbook |
| rinpol | 1014.00 | NIST Webbook |
| rinpol | 1009.00 | NIST Webbook |
| rinpol | 996.00 | NIST Webbook |
| rinpol | 991.00 | NIST Webbook |
| rinpol | 987.00 | NIST Webbook |
| rinpol | 1009.00 | NIST Webbook |
| rinpol | 1024.00 | NIST Webbook |
| rinpol | 1010.00 | NIST Webbook |
| rinpol | 998.00 | NIST Webbook |
| rinpol | 1013.00 | NIST Webbook |
| rinpol | 1004.00 | NIST Webbook |
| rinpol | 1004.00 | NIST Webbook |
| rinpol | 960.00 | NIST Webbook |
| rinpol | 970.00 | NIST Webbook |
| rinpol | 1046.00 | NIST Webbook |
| rinpol | 1008.00 | NIST Webbook |
| ripol | 1420.00 | NIST Webbook |
| ripol | 1483.20 | NIST Webbook |
| ripol | 1438.00 | NIST Webbook |
| ripol | 1438.00 | NIST Webbook |
| ripol | 1471.00 | NIST Webbook |
| ripol | 1438.00 | NIST Webbook |
| ripol | 1449.00 | NIST Webbook |
| ripol | 1449.00 | NIST Webbook |
| ripol | 1450.00 | NIST Webbook |
| ripol | 1446.09 | NIST Webbook |
| ripol | 1450.00 | NIST Webbook |
| ripol | 1446.00 | NIST Webbook |
| ripol | 1453.00 | NIST Webbook |

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|---|---|---|---|
| ripol | 1420.00 | | NIST Webbook |
| ripol | 1495.00 | | NIST Webbook |
| ripol | 1436.00 | | NIST Webbook |
| ripol | 1436.00 | | NIST Webbook |
| ripol | 1434.00 | | NIST Webbook |
| ss | 175.41 | J/mol×K | NIST Webbook |
| tb | 447.60 ± 0.50 | K | NIST Webbook |
| tb | 446.85 ± 0.70 | K | NIST Webbook |
| tb | 447.30 ± 0.50 | K | NIST Webbook |
| tb | 447.75 ± 0.30 | K | NIST Webbook |
| tb | 446.85 | K | KDB |
| tb | 447.20 | K | NIST Webbook |
| tb | 447.27 ± 0.07 | K | NIST Webbook |
| tc | 674.86 | K | Joback Method |
| tf | 326.41 | K | Aqueous Solubility Prediction Method |
| tf | 326.35 | K | KDB |
| tt | 326.15 ± 0.01 | K | NIST Webbook |
| tt | 326.16 | K | KDB |
| vc | 0.361 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 190.77 | J/mol×K | 674.86 | Joback Method |
| cpg | 178.92 | J/mol×K | 597.64 | Joback Method |
| cpg | 172.26 | J/mol×K | 559.03 | Joback Method |
| cpg | 165.09 | J/mol×K | 520.42 | Joback Method |
| cpg | 157.36 | J/mol×K | 481.81 | Joback Method |
| cpg | 149.05 | J/mol×K | 443.20 | Joback Method |
| cpg | 185.08 | J/mol×K | 636.25 | Joback Method |
| cpl | 182.71 | J/mol×K | 351.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 182.22 | J/mol×K | 349.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |

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|---|---|---|---|---|
| cpl | 179.81 | J/mol×K | 339.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 181.24 | J/mol×K | 345.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 180.76 | J/mol×K | 343.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 180.28 | J/mol×K | 341.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 183.21 | J/mol×K | 353.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 179.35 | J/mol×K | 337.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 178.89 | J/mol×K | 335.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 178.43 | J/mol×K | 333.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 177.98 | J/mol×K | 331.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |

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|---|---|---|---|---|
| cpl | 181.73 | J/mol×K | 347.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 177.09 | J/mol×K | 327.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cpl | 177.53 | J/mol×K | 329.15 | Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes |
| cps | 98.00 | J/mol×K | 180.00 | NIST Webbook |
| cps | 147.76 | J/mol×K | 298.15 | NIST Webbook |
| cps | 142.70 | J/mol×K | 298.15 | NIST Webbook |
| cps | 172.00 | J/mol×K | 299.80 | NIST Webbook |
| cps | 147.60 | J/mol×K | 298.00 | NIST Webbook |
| dvisc | 0.0003668 | Pa×s | 412.03 | Joback Method |
| dvisc | 0.0004656 | Pa×s | 380.85 | Joback Method |
| dvisc | 0.0006166 | Pa×s | 349.68 | Joback Method |
| dvisc | 0.0008628 | Pa×s | 318.51 | Joback Method |
| dvisc | 0.0012985 | Pa×s | 287.33 | Joback Method |
| dvisc | 0.0002989 | Pa×s | 443.20 | Joback Method |
| dvisc | 0.0021588 | Pa×s | 256.16 | Joback Method |
| hfust | 18.19 | kJ/mol | 326.20 | NIST Webbook |
| hfust | 18.16 | kJ/mol | 326.00 | NIST Webbook |
| hfust | 18.05 | kJ/mol | 326.15 | NIST Webbook |
| hfust | 18.16 | kJ/mol | 326.00 | NIST Webbook |
| hfust | 18.14 | kJ/mol | 326.05 | NIST Webbook |
| hfust | 18.16 | kJ/mol | 326.00 | NIST Webbook |
| hfust | 17.91 | kJ/mol | 192.50 | NIST Webbook |
| hsubt | 63.00 ± 0.40 | kJ/mol | 318.00 | NIST Webbook |
| hsubt | 64.80 ± 0.80 | kJ/mol | 302.00 | NIST Webbook |
| hsubt | 64.80 ± 0.40 | kJ/mol | 303.00 | NIST Webbook |
| hsubt | 65.40 | kJ/mol | 363.00 | NIST Webbook |
| hsubt | 53.10 | kJ/mol | 285.50 | NIST Webbook |
| hsubt | 56.90 | kJ/mol | 275.50 | NIST Webbook |
| hvapt | 44.20 | kJ/mol | 403.00 | NIST Webbook |
| hvapt | 45.00 | kJ/mol | 394.50 | NIST Webbook |
| hvapt | 46.40 | kJ/mol | 326.00 | NIST Webbook |
| sfust | 55.60 | J/mol×K | 326.05 | NIST Webbook |

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|---|---|---|---|---|
| sfust | 55.70 | J/mol×K | 326.00 | NIST Webbook |
| sfust | 55.30 | J/mol×K | 326.15 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.47073e+01 |
| Coeff. B | -4.15642e+03 |
| Coeff. C | -3.53240e+01 |
| Temperature range (K), min. | 323.57 |
| Temperature range (K), max. | 477.69 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 8.13197e+01 |
| Coeff. B | -8.43460e+03 |
| Coeff. C | -9.63023e+00 |
| Coeff. D | 4.66574e-06 |
| Temperature range (K), min. | 326.14 |
| Temperature range (K), max. | 684.75 |

# Sources

**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

**Estimated Solubility Method:** http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

**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 Vapor Pressure Data:** https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1679

**Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes:** https://www.doi.org/10.1021/je600573w

**Prediction of Henry's Law Constants Using Internal Standards with Benchmark Values:** https://www.doi.org/10.1021/je3010535

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**KDB:** https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1679

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C106467&Units=SI

**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 |
| **cpl:** | Liquid phase heat capacity |
| **cps:** | Solid phase heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfpi:** | Enthalpy of formation of positive ion at standard conditions |
| **hfpiz:** | Enthalpy of formation of positive ion at 0K |
| **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 |
| **nfpaf:** | NFPA Fire Rating |
| **nfpah:** | NFPA Health Rating |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **sfust:** | Entropy of fusion at a given temperature |
| **ss:** | Solid phase molar entropy at standard conditions |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tt:** | Triple Point Temperature |
| **vc:** | Critical Volume |

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