# Propane, 1,2,3-trichloro-

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|---|---|
| **Other names:** | 1,2,3-Trichloropropane |
| | ALLYL TRICHLORIDE |
| | GLYCEROL TRICHLOROHYDRIN |
| | Glyceryl trichlorohydrin |
| | NCI-C60220 |
| | NSC 35403 |
| | Trichlorohydrin |
| **Inchi:** | InChI=1S/C3H5Cl3/c4-1-3(6)2-5/h3H,1-2H2 |
| **InchiKey:** | CFXQEHVMCRXUSD-UHFFFAOYSA-N |
| **Formula:** | C3H5Cl3 |
| **SMILES:** | ClCC(Cl)CCl |
| **Mol. weight [g/mol]:** | 147.43 |
| **CAS:** | 96-18-4 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.3100 | | KDB |
| chl | -1735.00 ± 0.80 | kJ/mol | NIST Webbook |
| chl | -1735.40 ± 1.30 | kJ/mol | NIST Webbook |
| chl | -1727.60 ± 1.80 | kJ/mol | NIST Webbook |
| dm | 1.60 | debye | KDB |
| gf | -97.85 | kJ/mol | KDB |
| hf | -185.90 | kJ/mol | KDB |
| hf | -183.00 ± 2.00 | kJ/mol | NIST Webbook |
| hfl | -230.00 ± 0.80 | kJ/mol | NIST Webbook |
| hfus | 12.59 | kJ/mol | Joback Method |
| hvap | 47.80 ± 0.10 | kJ/mol | NIST Webbook |
| log10ws | -1.92 | | Aqueous Solubility Prediction Method |
| logp | 2.071 | | Crippen Method |
| mcvol | 89.850 | ml/mol | McGowan Method |
| nfpaf | %!d(float64=2) | | KDB |
| nfpah | %!d(float64=3) | | KDB |
| pc | 3950.00 | kPa | KDB |
| rinpol | 890.00 | | NIST Webbook |
| rinpol | 938.00 | | NIST Webbook |
| rinpol | 899.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 945.00 | | NIST Webbook |
| rinpol | 899.00 | | NIST Webbook |
| rinpol | 924.00 | | NIST Webbook |
| rinpol | 883.00 | | NIST Webbook |
| rinpol | 910.00 | | NIST Webbook |
| rinpol | 910.00 | | NIST Webbook |
| rinpol | 878.40 | | NIST Webbook |
| ripol | 1455.00 | | NIST Webbook |
| ripol | 1420.00 | | NIST Webbook |
| tb | 429.00 | K | KDB |
| tc | 651.00 | K | KDB |
| tf | 258.50 | K | KDB |
| tf | 258.58 | K | Aqueous Solubility Prediction Method |
| tf | 258.45 | K | NIST Webbook |
| tf | 259.40 ± 0.60 | K | NIST Webbook |
| vc | 0.348 | m3/kmol | KDB |
| zc | 0.2539560 | | KDB |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 156.39 | J/mol×K | 543.44 | Joback Method |
| cpg | 130.24 | J/mol×K | 379.89 | Joback Method |
| cpg | 136.05 | J/mol×K | 412.60 | Joback Method |
| cpg | 141.56 | J/mol×K | 445.31 | Joback Method |
| cpg | 146.78 | J/mol×K | 478.02 | Joback Method |
| cpg | 151.72 | J/mol×K | 510.73 | Joback Method |
| cpg | 160.80 | J/mol×K | 576.15 | Joback Method |
| cpl | 183.60 | J/mol×K | 298.00 | NIST Webbook |
| cpl | 172.80 | J/mol×K | 298.00 | NIST Webbook |
| dvisc | 0.0003904 | Pa×s | 379.89 | Joback Method |
| dvisc | 0.0061584 | Pa×s | 198.33 | Joback Method |
| dvisc | 0.0028685 | Pa×s | 228.59 | Joback Method |
| dvisc | 0.0015974 | Pa×s | 258.85 | Joback Method |
| dvisc | 0.0010055 | Pa×s | 289.11 | Joback Method |
| dvisc | 0.0006910 | Pa×s | 319.37 | Joback Method |
| dvisc | 0.0005067 | Pa×s | 349.63 | Joback Method |
| hvapt | 46.80 | kJ/mol | 356.50 | NIST Webbook |
| hvapt | 38.41 | kJ/mol | 429.00 | KDB |
| hvapt | 43.00 | kJ/mol | 407.00 | NIST Webbook |

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|---|---|---|---|---|
| hvapt | 43.00 | kJ/mol | 395.00 | NIST Webbook |
| hvapt | 48.00 ± 1.00 | kJ/mol | 293.00 | NIST Webbook |
| rhol | 1389.00 | kg/m3 | 293.00 | KDB |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.51253e+01 |
| Coeff. B | -3.86982e+03 |
| Coeff. C | -6.06900e+01 |
| Temperature range (K), min. | 321.50 |
| Temperature range (K), max. | 456.34 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 6.16678e+01 |
| Coeff. B | -7.35551e+03 |
| Coeff. C | -6.65548e+00 |
| Coeff. D | 2.27606e-06 |
| Temperature range (K), min. | 258.45 |
| Temperature range (K), max. | 652.00 |

# Sources

**KDB Vapor Pressure Data:** https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1584

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

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

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

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

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

**KDB:** https://www.cheric.org/files/research/kdb/mol/mol1584.mol

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C96184&Units=SI

**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase heat capacity |
| **dm:** | Dipole Moment |
| **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 |
| **nfpaf:** | NFPA Fire Rating |
| **nfpah:** | NFPA Health Rating |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **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 |
| **zc:** | Critical Compressibility |

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