# Phosgene

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|---|---|
| **Other names:** | CARBON DICHLORIDE OXIDE |
| | CARBON OXYCHLORIDE |
| | CARBONYL DICHLORIDE |
| | CG |
| | COCl2 |
| | Carbone (oxychlorure de) |
| | Carbonic chloride |
| | Carbonic dichloride |
| | Carbonio (ossicloruro di) |
| | Carbonyl chloride |
| | Carbonylchlorid |
| | Chloroformyl chloride |
| | Dichloroformaldehyde |
| | Fosgeen |
| | Fosgen |
| | Fosgene |
| | Koolstofoxychloride |
| | NCI-C60219 |
| | Phosgen |
| | Rcra waste number P095 |
| | UN 1076 |
| **Inchi:** | InChI=1S/CCl2O/c2-1(3)4 |
| **InchiKey:** | YGYAWVDWMABLBF-UHFFFAOYSA-N |
| **Formula:** | CCl2O |
| **SMILES:** | O=C(Cl)Cl |
| **Mol. weight [g/mol]:** | 98.92 |
| **CAS:** | 75-44-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.2050 | | KDB |
| chg | -108.60 ± 0.42 | kJ/mol | NIST Webbook |
| dm | 1.10 | debye | KDB |
| gf | -206.90 | kJ/mol | KDB |
| hf | -221.10 | kJ/mol | KDB |
| hf | -219.10 ± 0.59 | kJ/mol | NIST Webbook |

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|---|---|---|---|
| hf | -209.50 ± 1.20 | kJ/mol | NIST Webbook |
| hf | -220.10 ± 0.96 | kJ/mol | NIST Webbook |
| hfus | 8.34 | kJ/mol | Joback Method |
| hvap | 33.34 | kJ/mol | Joback Method |
| ie | 11.20 | eV | NIST Webbook |
| ie | 11.55 ± 0.02 | eV | NIST Webbook |
| ie | 11.70 | eV | NIST Webbook |
| ie | 11.84 | eV | NIST Webbook |
| log10ws | -1.30 | | Crippen Method |
| logp | 1.584 | | Crippen Method |
| mcvol | 51.000 | ml/mol | McGowan Method |
| pc | 5674.00 | kPa | KDB |
| rinpol | 425.00 | | NIST Webbook |
| rinpol | 425.00 | | NIST Webbook |
| rinpol | 416.00 | | NIST Webbook |
| sl | 192.80 | J/mol×K | NIST Webbook |
| sl | 198.11 | J/mol×K | NIST Webbook |
| tb | 280.71 | K | KDB |
| tc | 455.15 | K | KDB |
| tf | 145.00 | K | KDB |
| tt | 139.19 ± 0.20 | K | NIST Webbook |
| tt | 145.37 ± 0.02 | K | NIST Webbook |
| tt | 145.37 ± 0.02 | K | NIST Webbook |
| tt | 142.09 ± 0.05 | K | NIST Webbook |
| vc | 0.190 | m3/kmol | KDB |
| zc | 0.2850230 | | KDB |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 67.23 | J/mol×K | 550.64 | Joback Method |
| cpg | 64.72 | J/mol×K | 484.10 | Joback Method |
| cpg | 66.02 | J/mol×K | 517.37 | Joback Method |
| cpg | 58.67 | J/mol×K | 351.01 | Joback Method |
| cpg | 60.32 | J/mol×K | 384.28 | Joback Method |
| cpg | 61.88 | J/mol×K | 417.55 | Joback Method |
| cpg | 63.34 | J/mol×K | 450.83 | Joback Method |
| cpl | 100.79 | J/mol×K | 280.00 | NIST Webbook |
| cpl | 102.59 | J/mol×K | 160.55 | NIST Webbook |
| dvisc | 0.0006616 | Pa×s | 304.27 | Joback Method |
| dvisc | 0.0005242 | Pa×s | 327.64 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0004284 | Pa×s | 351.01 | Joback Method |
| dvisc | 0.0011966 | Pa×s | 257.54 | Joback Method |
| dvisc | 0.0028142 | Pa×s | 210.80 | Joback Method |
| dvisc | 0.0017584 | Pa×s | 234.17 | Joback Method |
| dvisc | 0.0008681 | Pa×s | 280.90 | Joback Method |
| hfust | 5.73 | kJ/mol | 145.30 | NIST Webbook |
| hfust | 5.74 | kJ/mol | 145.37 | NIST Webbook |
| hvapt | 24.50 | kJ/mol | 374.00 | NIST Webbook |
| hvapt | 24.40 | kJ/mol | 430.50 | NIST Webbook |
| hvapt | 27.00 | kJ/mol | 231.50 | NIST Webbook |
| hvapt | 24.40 | kJ/mol | 280.71 | NIST Webbook |
| hvapt | 24.50 | kJ/mol | 310.50 | NIST Webbook |
| hvapt | 25.70 | kJ/mol | 260.50 | NIST Webbook |
| hvapt | 25.80 | kJ/mol | 226.50 | NIST Webbook |
| rhol | 1381.00 | kg/m3 | 293.00 | KDB |
| sfust | 39.46 | J/mol×K | 145.37 | NIST Webbook |
| svapt | 86.93 | J/mol×K | 280.71 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.44269e+01 |
| Coeff. B | -2.44909e+03 |
| Coeff. C | -3.10200e+01 |
| Temperature range (K), min. | 145.37 |
| Temperature range (K), max. | 455.00 |

# Sources

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

**KDB:** https://www.cheric.org/files/research/kdb/mol/mol1764.mol

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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C75445&Units=SI

**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

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **chg:** | Standard gas 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 |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion 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 |
| **rhol:** | Liquid Density |
| **rinpol:** | Non-polar retention indices |
| **sfust:** | Entropy of fusion at a given temperature |
| **sl:** | Liquid phase molar entropy at standard conditions |
| **svapt:** | Entropy of vaporization at a given temperature |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tt:** | Triple Point Temperature |
| **vc:** | Critical Volume |
| **zc:** | Critical Compressibility |