# 2,4-Dichloro-1-vinylbenzene

**Other names:** 2,4-dichlorostyrene
**Inchi:** InChI=1S/C8H6Cl2/c1-2-6-3-4-7(9)5-8(6)10/h2-5H,1H2
**InchiKey:** OMNYXCUDBQKCMU-UHFFFAOYSA-N
**Formula:** C8H6Cl2
**SMILES:** C=Cc1ccc(Cl)cc1Cl
**Mol. weight [g/mol]:** 173.04
**CAS:** 2123-27-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 173.61 | kJ/mol | Joback Method |
| hf | 99.09 | kJ/mol | Joback Method |
| hfus | 16.85 | kJ/mol | Joback Method |
| hvap | 45.10 | kJ/mol | Joback Method |
| log10ws | -3.67 | | Crippen Method |
| logp | 3.636 | | Crippen Method |
| mcvol | 120.000 | ml/mol | McGowan Method |
| pc | 3392.03 | kPa | Joback Method |
| tb | 490.62 | K | Joback Method |
| tc | 721.44 | K | Joback Method |
| tf | 289.46 | K | Joback Method |
| vc | 0.455 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 258.72 | J/mol×K | 721.44 | Joback Method |
| cpg | 209.24 | J/mol×K | 490.62 | Joback Method |
| cpg | 219.01 | J/mol×K | 529.09 | Joback Method |
| cpg | 228.14 | J/mol×K | 567.56 | Joback Method |
| cpg | 236.64 | J/mol×K | 606.03 | Joback Method |
| cpg | 244.54 | J/mol×K | 644.50 | Joback Method |
| cpg | 251.90 | J/mol×K | 682.97 | Joback Method |
| dvisc | 0.0002653 | Pa×s | 490.62 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0016081 | Pa×s | 289.46 | Joback Method |
| dvisc | 0.0010190 | Pa×s | 322.99 | Joback Method |
| dvisc | 0.0007036 | Pa×s | 356.51 | Joback Method |
| dvisc | 0.0005178 | Pa×s | 390.04 | Joback Method |
| dvisc | 0.0004000 | Pa×s | 423.57 | Joback Method |
| dvisc | 0.0003209 | Pa×s | 457.09 | Joback Method |
| hvapt | 55.00 | kJ/mol | 412.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.53430e+01 |
| Coeff. B | -4.99971e+03 |
| Coeff. C | -3.73980e+01 |
| Temperature range (K), min. | 326.00 |
| Temperature range (K), max. | 535.80 |

# Sources

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

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

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

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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C2123275&Units=SI

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

# Legend

**cpg:** Ideal gas heat capacity

**dvisc:** Dynamic viscosity

**gf:** Standard Gibbs free energy of formation

**hf:** 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 |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |