# Propene, 3,3-dichloro-2-methyl-

**Other names:** 3,3-dichloro-2-methyl-1-propene
**Inchi:** InChI=1S/C4H6Cl2/c1-3(2)4(5)6/h4H,1H2,2H3
**InchiKey:** IBOBCGSJCSKTKP-UHFFFAOYSA-N
**Formula:** C4H6Cl2
**SMILES:** C=C(C)C(Cl)Cl
**Mol. weight [g/mol]:** 125.00
**CAS:** 22227-75-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 35.79 | kJ/mol | Joback Method |
| hf | -47.01 | kJ/mol | Joback Method |
| hfus | 8.40 | kJ/mol | Joback Method |
| hvap | 32.29 | kJ/mol | Joback Method |
| log10ws | -2.26 | | Crippen Method |
| logp | 2.366 | | Crippen Method |
| mcvol | 87.400 | ml/mol | McGowan Method |
| pc | 3805.69 | kPa | Joback Method |
| rinpol | 726.00 | | NIST Webbook |
| tb | 361.90 | K | Joback Method |
| tc | 556.48 | K | Joback Method |
| tf | 163.96 | K | Joback Method |
| vc | 0.334 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 128.38 | J/mol×K | 361.90 | Joback Method |
| cpg | 135.37 | J/mol×K | 394.33 | Joback Method |
| cpg | 142.00 | J/mol×K | 426.76 | Joback Method |
| cpg | 148.26 | J/mol×K | 459.19 | Joback Method |
| cpg | 154.19 | J/mol×K | 491.62 | Joback Method |
| cpg | 159.79 | J/mol×K | 524.05 | Joback Method |
| cpg | 165.08 | J/mol×K | 556.48 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.41662e+01 |
| Coeff. B | -3.28659e+03 |
| Coeff. C | -4.71100e+01 |
| Temperature range (K), min. | 283.92 |
| Temperature range (K), max. | 418.28 |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C22227754&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 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |

| | |
|---|---|
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |