# Acetonitrile, trichloro-

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|---|---|
| **Other names:** | 2,2,2-trichloroacetonitrile |
| | Acetonitrile, 2,2,2-trichloro- |
| | CCl3CN |
| | Cyanotrichloromethane |
| | NSC 66405 |
| | Nitrile trichloracetique |
| | Trichlor-acetonitril |
| | Trichlormethylkyanid |
| | Trichloroacetonitrile |
| | Trichloroethanenitrile |
| | Trichloromethyl cyanide |
| | Trichloromethylnitrile |
| | Trichlouracetonitril |
| | Tritox |
| **Inchi:** | InChI=1S/C2Cl3N/c3-2(4,5)1-6 |
| **InchiKey:** | DRUIESSIVFYOMK-UHFFFAOYSA-N |
| **Formula:** | C2Cl3N |
| **SMILES:** | N#CC(Cl)(Cl)Cl |
| **Mol. weight [g/mol]:** | 144.39 |
| **CAS:** | 545-06-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 723.20 | kJ/mol | NIST Webbook |
| basg | 692.60 | kJ/mol | NIST Webbook |
| ea | 0.30 ± 0.20 | eV | NIST Webbook |
| gf | 66.19 | kJ/mol | Joback Method |
| hf | 24.30 | kJ/mol | Joback Method |
| hfus | 7.62 | kJ/mol | Joback Method |
| hvap | 42.38 | kJ/mol | Joback Method |
| ie | 11.96 | eV | NIST Webbook |
| ie | 11.89 | eV | NIST Webbook |
| log10ws | -2.17 | | Aqueous Solubility Prediction Method |
| log10ws | -2.17 | | Estimated Solubility Method |
| logp | 1.880 | | Crippen Method |

| | | | |
|---|---|---|---|
| mcvol | 77.140 | ml/mol | McGowan Method |
| pc | 4288.66 | kPa | Joback Method |
| rinpol | 668.00 | | NIST Webbook |
| rinpol | 662.00 | | NIST Webbook |
| rinpol | 668.00 | | NIST Webbook |
| rinpol | 662.00 | | NIST Webbook |
| tb | 357.00 ± 2.00 | K | NIST Webbook |
| tb | 356.70 | K | NIST Webbook |
| tc | 690.30 | K | Joback Method |
| tf | 230.48 | K | Aqueous Solubility Prediction Method |
| vc | 0.309 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 107.90 | J/mol×K | 456.30 | Joback Method |
| cpg | 110.75 | J/mol×K | 495.30 | Joback Method |
| cpg | 113.21 | J/mol×K | 534.30 | Joback Method |
| cpg | 115.31 | J/mol×K | 573.30 | Joback Method |
| cpg | 117.08 | J/mol×K | 612.30 | Joback Method |
| cpg | 118.57 | J/mol×K | 651.30 | Joback Method |
| cpg | 119.81 | J/mol×K | 690.30 | Joback Method |
| hvapt | 35.10 | kJ/mol | 323.00 | NIST Webbook |
| hvapt | 34.70 | kJ/mol | 322.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.47887e+01 |
| Coeff. B | -3.31205e+03 |
| Coeff. C | -3.31930e+01 |
| Temperature range (K), min. | 257.15 |
| Temperature range (K), max. | 382.67 |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C545062&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 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **cpg:** | Ideal gas heat capacity |
| **ea:** | Electron affinity |
| **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 |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |