# 1,2-Benzenedicarbonitrile, 3,4,5,6-tetrachloro-

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|---|---|
| **Other names:** | Phthalonitrile, tetrachloro- |
| | Tetrachlorophthalodinitrile |
| | Tetrachlorophthalonitrile |
| | 3,4,5,6-Tetrachlorophthalonitrile |
| | o-Phthalodinitrile, tetrachloro- |
| | o-Tcpn |
| | o-Tetrachlorophthalodinitrile |
| | 3,4,5,6-tetrachlorobenzene-1,2-dicarbonitrile |
| **Inchi:** | InChI=1S/C8Cl4N2/c9-5-3(1-13)4(2-14)6(10)8(12)7(5)11 |
| **InchiKey:** | OQHXZZGZASQSOB-UHFFFAOYSA-N |
| **Formula:** | C8Cl4N2 |
| **SMILES:** | N#Cc1c(Cl)c(Cl)c(Cl)c(Cl)c1C#N |
| **Mol. weight [g/mol]:** | 265.91 |
| **CAS:** | 1953-99-7 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 299.38 | kJ/mol | Joback Method |
| hf | 237.53 | kJ/mol | Joback Method |
| hfus | 28.37 | kJ/mol | Joback Method |
| hvap | 77.48 | kJ/mol | Joback Method |
| log10ws | -4.92 | | Crippen Method |
| logp | 4.044 | | Crippen Method |
| mcvol | 151.540 | ml/mol | McGowan Method |
| pc | 2690.21 | kPa | Joback Method |
| tb | 787.90 | K | Joback Method |
| tc | 1048.40 | K | Joback Method |
| tf | 518.60 | K | Joback Method |
| vc | 0.624 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 267.96 | J/mol×K | 787.90 | Joback Method |

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|---|---|---|---|---|
| cpg | 272.09 | J/mol×K | 831.32 | Joback Method |
| cpg | 275.82 | J/mol×K | 874.73 | Joback Method |
| cpg | 279.15 | J/mol×K | 918.15 | Joback Method |
| cpg | 282.09 | J/mol×K | 961.57 | Joback Method |
| cpg | 284.64 | J/mol×K | 1004.98 | Joback Method |
| cpg | 286.81 | J/mol×K | 1048.40 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1953997&Units=SI |
| **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 |

# Legend

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