# Benzonitrile, pentachloro-

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|---|---|
| **Other names:** | Pentachlorobenzonitrile |
| | 2,3,4,5,6-Pentachlorobenzonitrile |
| | Pentachlorocyanobenzene |
| | Pentachlorobenzonitryl |
| **Inchi:** | InChI=1S/C7Cl5N/c8-3-2(1-13)4(9)6(11)7(12)5(3)10 |
| **InchiKey:** | INICGXSKJYKEIV-UHFFFAOYSA-N |
| **Formula:** | C7Cl5N |
| **SMILES:** | N#Cc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl |
| **Mol. weight [g/mol]:** | 275.35 |
| **CAS:** | 20925-85-3 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 145.85 | kJ/mol | Joback Method |
| hf | 77.55 | kJ/mol | Joback Method |
| hfus | 28.47 | kJ/mol | Joback Method |
| hvap | 69.17 | kJ/mol | Joback Method |
| log10ws | -5.25 | | Crippen Method |
| logp | 4.825 | | Crippen Method |
| mcvol | 148.310 | ml/mol | McGowan Method |
| pc | 2940.89 | kPa | Joback Method |
| tb | 700.37 | K | Joback Method |
| tc | 959.39 | K | Joback Method |
| tf | 472.26 | K | Joback Method |
| vc | 0.591 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 241.74 | J/mol×K | 700.37 | Joback Method |
| cpg | 246.08 | J/mol×K | 743.54 | Joback Method |
| cpg | 250.06 | J/mol×K | 786.71 | Joback Method |
| cpg | 253.68 | J/mol×K | 829.88 | Joback Method |
| cpg | 256.95 | J/mol×K | 873.05 | Joback Method |

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|---|---|---|---|---|
| cpg | 259.87 | J/mol×K | 916.22 | Joback Method |
| cpg | 262.45 | J/mol×K | 959.39 | Joback Method |

# Sources

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|---|---|
| **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=C20925853&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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