# 1,1'-Biphenyl, 2,2',3,4,5-pentachloro-

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|---|---|
| **Other names:** | 1,2,3,4-tetrachloro-5-(2-chlorophenyl)benzene |
| | 2,2',3,4,5-Pentachloro-1,1'-biphenyl |
| | 2,2',3,4,5-Pentachlorobiphenyl |
| | PCB 86 |
| **Inchi:** | InChI=1S/C12H5Cl5/c13-8-4-2-1-3-6(8)7-5-9(14)11(16)12(17)10(7)15/h1-5H |
| **InchiKey:** | AIURIRUDHVDRFQ-UHFFFAOYSA-N |
| **Formula:** | C12H5Cl5 |
| **SMILES:** | Clc1ccccc1-c1cc(Cl)c(Cl)c(Cl)c1Cl |
| **Mol. weight [g/mol]:** | 326.44 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.5243 | | Cheméo Relay (1.0) |
| gf | 167.18 | kJ/mol | Joback Method |
| hf | 84.95 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 33.96 | kJ/mol | Joback Method |
| hvap | 96.60 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.51 | eV | Cheméo Relay (1.0) |
| log10ws | -7.21 | | Aqueous Solubility Prediction Method |
| logp | 6.621 | | Crippen Method |
| mcvol | 193.620 | ml/mol | McGowan Method |
| pc | 2581.96 | kPa | Joback Method |
| tb | 636.76 | K | Cheméo Relay (1.0) |
| tc | 921.56 | K | Cheméo Relay (1.0) |
| tf | 364.93 | K | Cheméo Relay (1.0) |
| vc | 0.703 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 385.50 | J/mol×K | 739.37 | Joback Method |
| cpg | 394.64 | J/mol×K | 784.18 | Joback Method |
| cpg | 402.91 | J/mol×K | 828.99 | Joback Method |

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|---|---|---|---|---|
| cpg | 410.38 | J/mol×K | 873.79 | Joback Method |
| cpg | 417.08 | J/mol×K | 918.60 | Joback Method |
| cpg | 423.09 | J/mol×K | 963.41 | Joback Method |
| cpg | 428.46 | J/mol×K | 1008.22 | Joback Method |
| dvisc | 0.0006694 | Pa×s | 490.04 | Joback Method |
| dvisc | 0.0004783 | Pa×s | 531.60 | Joback Method |
| dvisc | 0.0003588 | Pa×s | 573.15 | Joback Method |
| dvisc | 0.0002798 | Pa×s | 614.71 | Joback Method |
| dvisc | 0.0002252 | Pa×s | 656.26 | Joback Method |
| dvisc | 0.0001860 | Pa×s | 697.82 | Joback Method |
| dvisc | 0.0001570 | Pa×s | 739.37 | Joback Method |

# Sources

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C55312691&Units=SI

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

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

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

# Legend

**af:** Acentric Factor
**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
**ie:** Ionization energy
**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