# 1,1'-Biphenyl, 2,2',4,4',6,6'-hexachloro-

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|---|---|
| **Other names:** | 2,2',4,4',6,6'-Hexachloro-1,1'-biphenyl |
| | 2,2',4,4',6,6'-Hexachlorobiphenyl |
| | 2,2',4,4',6,6'-Hexachlorodiphenyl |
| | 2,2',4,4',6,6'-PCB |
| | 2,4,6,2',4',6'-Hexachlorobiphenyl |
| | Biphenyl, 2,2',4,4',6,6'-hexachloro- |
| | PCB 155 |
| **Inchi:** | InChI=1S/C12H4Cl6/c13-5-1-7(15)11(8(16)2-5)12-9(17)3-6(14)4-10(12)18/h1-4H |
| **InchiKey:** | ICOAEPDGFWLUTI-UHFFFAOYSA-N |
| **Formula:** | C12H4Cl6 |
| **SMILES:** | Clc1cc(Cl)c(-c2c(Cl)cc(Cl)cc2Cl)c(Cl)c1 |
| **Mol. weight [g/mol]:** | 360.88 |
| **CAS:** | 33979-03-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 145.62 | kJ/mol | Joback Method |
| hf | 18.79 | kJ/mol | Joback Method |
| hfus | 37.77 | kJ/mol | Joback Method |
| hvap | 77.14 | kJ/mol | Joback Method |
| log10ws | -8.71 | | Estimated Solubility Method |
| log10ws | -8.41 | | Aqueous Solubility Prediction Method |
| logp | 7.274 | | Crippen Method |
| mcvol | 205.860 | ml/mol | McGowan Method |
| pc | 2450.74 | kPa | Joback Method |
| rinpol | 2026.00 | | NIST Webbook |
| rinpol | 2045.00 | | NIST Webbook |
| rinpol | 2026.00 | | NIST Webbook |
| rinpol | 2026.00 | | NIST Webbook |
| rinpol | 2045.00 | | NIST Webbook |
| tb | 781.78 | K | Joback Method |
| tc | 1052.68 | K | Joback Method |
| tf | 386.70 ± 0.20 | K | NIST Webbook |
| vc | 0.785 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 401.07 | J/mol×K | 781.78 | Joback Method |
| cpg | 409.07 | J/mol×K | 826.93 | Joback Method |
| cpg | 416.26 | J/mol×K | 872.08 | Joback Method |
| cpg | 422.71 | J/mol×K | 917.23 | Joback Method |
| cpg | 428.46 | J/mol×K | 962.38 | Joback Method |
| cpg | 433.56 | J/mol×K | 1007.53 | Joback Method |
| cpg | 438.05 | J/mol×K | 1052.68 | Joback Method |
| dvisc | 0.0003981 | Pa×s | 574.03 | Joback Method |
| dvisc | 0.0005388 | Pa×s | 532.48 | Joback Method |
| dvisc | 0.0003063 | Pa×s | 615.58 | Joback Method |
| dvisc | 0.0002437 | Pa×s | 657.13 | Joback Method |
| dvisc | 0.0001992 | Pa×s | 698.68 | Joback Method |
| dvisc | 0.0001666 | Pa×s | 740.23 | Joback Method |
| dvisc | 0.0001419 | Pa×s | 781.78 | Joback Method |
| hfust | 17.50 | kJ/mol | 386.70 | NIST Webbook |
| hfust | 17.50 | kJ/mol | 386.70 | NIST Webbook |
| hsubt | 103.40 ± 2.30 | kJ/mol | 283.00 | NIST Webbook |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C33979032&Units=SI
**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
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions

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|---|---|
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |