# 1,1'-Biphenyl, 2,3,4'-Trichloro-

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|---|---|
| **Other names:** | 1,2-dichloro-3-(4-chlorophenyl)benzene |
| | 2,3,4'-PCB |
| | 2,3,4'-Trichlorobiphenyl |
| | PCB 22 |
| **Inchi:** | InChI=1S/C12H7Cl3/c13-9-6-4-8(5-7-9)10-2-1-3-11(14)12(10)15/h1-7H |
| **InchiKey:** | ZMHWQAHZKUPENF-UHFFFAOYSA-N |
| **Formula:** | C12H7Cl3 |
| **SMILES:** | Clc1ccc(-c2cccc(Cl)c2Cl)cc1 |
| **Mol. weight [g/mol]:** | 257.54 |
| **CAS:** | 38444-85-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -5617.23 | kJ/mol | NIST Webbook |
| gf | 210.30 | kJ/mol | Joback Method |
| hf | 100.42 | kJ/mol | Joback Method |
| hfus | 26.34 | kJ/mol | Joback Method |
| hvap | 62.00 | kJ/mol | Joback Method |
| log10ws | -6.26 | | Estimated Solubility Method |
| log10ws | -6.26 | | Aqueous Solubility Prediction Method |
| logp | 5.314 | | Crippen Method |
| mcvol | 169.140 | ml/mol | McGowan Method |
| pc | 2878.12 | kPa | Joback Method |
| rinpol | 1929.00 | | NIST Webbook |
| rinpol | 1932.00 | | NIST Webbook |
| rinpol | 1932.00 | | NIST Webbook |
| rinpol | 1896.00 | | NIST Webbook |
| rinpol | 1889.00 | | NIST Webbook |
| rinpol | 1848.00 | | NIST Webbook |
| rinpol | 1932.00 | | NIST Webbook |
| tb | 654.55 | K | Joback Method |
| tc | 917.95 | K | Joback Method |
| tf | 405.16 | K | Joback Method |
| vc | 0.638 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 349.20 | J/mol×K | 654.55 | Joback Method |
| cpg | 360.92 | J/mol×K | 698.45 | Joback Method |
| cpg | 371.61 | J/mol×K | 742.35 | Joback Method |
| cpg | 381.33 | J/mol×K | 786.25 | Joback Method |
| cpg | 390.14 | J/mol×K | 830.15 | Joback Method |
| cpg | 398.13 | J/mol×K | 874.05 | Joback Method |
| cpg | 405.36 | J/mol×K | 917.95 | Joback Method |
| dvisc | 0.0010725 | Pa×s | 405.16 | Joback Method |
| dvisc | 0.0006985 | Pa×s | 446.73 | Joback Method |
| dvisc | 0.0004893 | Pa×s | 488.29 | Joback Method |
| dvisc | 0.0003625 | Pa×s | 529.86 | Joback Method |
| dvisc | 0.0002805 | Pa×s | 571.42 | Joback Method |
| dvisc | 0.0002248 | Pa×s | 612.99 | Joback Method |
| dvisc | 0.0001852 | Pa×s | 654.55 | Joback Method |

# Sources

**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
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C38444858&Units=SI

# Legend

**chs:** Standard solid enthalpy of combustion
**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

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|---|---|
| **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 |