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

**Other names:** 2,3,4-Trichloro-1,1'-biphenyl
2,3,4-Trichlorobiphenyl
PCB 21
**Inchi:** InChI=1S/C12H7Cl3/c13-10-7-6-9(11(14)12(10)15)8-4-2-1-3-5-8/h1-7H
**InchiKey:** IUYHQGMDSZOPDZ-UHFFFAOYSA-N
**Formula:** C12H7Cl3
**SMILES:** Clc1ccc(-c2ccccc2)c(Cl)c1Cl
**Mol. weight [g/mol]:** 257.54
**CAS:** 55702-46-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| 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 | -6.13 | | Crippen Method |
| logp | 5.314 | | Crippen Method |
| mcvol | 169.140 | ml/mol | McGowan Method |
| pc | 2878.12 | kPa | Joback Method |
| rinpol | 1918.00 | | NIST Webbook |
| rinpol | 1877.00 | | 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:** | 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=C55702460&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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

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