# 1,1'-Biphenyl, 2,5-dichloro-

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|---|---|
| **Other names:** | 2,5-Dichloro-1,1'-biphenyl |
| | 2,5-Dichlorobiphenyl |
| | Biphenyl, 2,5-dichloro- |
| | PCB 9 |
| **Inchi:** | InChI=1S/C12H8Cl2/c13-10-6-7-12(14)11(8-10)9-4-2-1-3-5-9/h1-8H |
| **InchiKey:** | KKQWHYGECTYFIA-UHFFFAOYSA-N |
| **Formula:** | C12H8Cl2 |
| **SMILES:** | Clc1ccc(Cl)c(-c2ccccc2)c1 |
| **Mol. weight [g/mol]:** | 223.10 |
| **CAS:** | 34883-39-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 231.86 | kJ/mol | Joback Method |
| hf | 127.63 | kJ/mol | Joback Method |
| hfus | 22.53 | kJ/mol | Joback Method |
| hvap | 76.80 ± 0.40 | kJ/mol | NIST Webbook |
| log10ws | -5.24 | | Aqueous Solubility Prediction Method |
| logp | 4.660 | | Crippen Method |
| mcvol | 156.900 | ml/mol | McGowan Method |
| pc | 3045.68 | kPa | Joback Method |
| rinpol | 1635.00 | | NIST Webbook |
| rinpol | 1635.00 | | NIST Webbook |
| rinpol | 1672.00 | | NIST Webbook |
| rinpol | 1656.00 | | NIST Webbook |
| rinpol | 1637.00 | | NIST Webbook |
| rinpol | 1637.00 | | NIST Webbook |
| rinpol | 1672.00 | | NIST Webbook |
| rinpol | 1628.00 | | NIST Webbook |
| rinpol | 1635.00 | | NIST Webbook |
| tb | 612.14 | K | Joback Method |
| tc | 871.88 | K | Joback Method |
| tf | 362.72 | K | Joback Method |
| vc | 0.590 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 391.60 | J/mol×K | 871.88 | Joback Method |
| cpg | 383.35 | J/mol×K | 828.59 | Joback Method |
| cpg | 374.26 | J/mol×K | 785.30 | Joback Method |
| cpg | 364.26 | J/mol×K | 742.01 | Joback Method |
| cpg | 353.28 | J/mol×K | 698.72 | Joback Method |
| cpg | 341.24 | J/mol×K | 655.43 | Joback Method |
| cpg | 328.07 | J/mol×K | 612.14 | Joback Method |
| dvisc | 0.0013975 | Pa×s | 362.72 | Joback Method |
| dvisc | 0.0001963 | Pa×s | 612.14 | Joback Method |
| dvisc | 0.0002417 | Pa×s | 570.57 | Joback Method |
| dvisc | 0.0003074 | Pa×s | 529.00 | Joback Method |
| dvisc | 0.0004074 | Pa×s | 487.43 | Joback Method |
| dvisc | 0.0005691 | Pa×s | 445.86 | Joback Method |
| dvisc | 0.0008516 | Pa×s | 404.29 | Joback Method |
| hvapt | 73.90 | kJ/mol | 368.00 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 444.20 | K | 2.00 | NIST Webbook |

# Sources

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

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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C34883391&Units=SI

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

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

# 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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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