

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

**Other names:** 2,3',4,5,5'-Pentachloro-1,1'-biphenyl; PCB 120.

**InChI:** InChI=1S/C12H5Cl5/c13-7-1-6(2-8(14)3-7)9-4-11(16)12(17)5-10(9)15/h1-5H

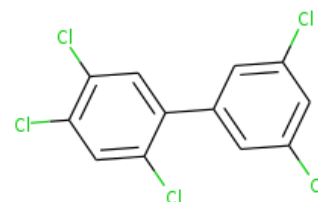
**InChI Key:** ZLGYJAIAPVCNF-UHFFFAOYSA-N

**Formula:** C12H5Cl5

**SMILES:** Clc1cc(Cl)cc(-c2cc(Cl)c(Cl)cc2Cl)c1

**Molecular Weight:** 326.43

**CAS:** 68194-12-7



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	167.18	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	46.00	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	33.96	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	72.09	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	6.62		Crippen Method
$P_c$	2581.96	kPa	Joback Method
$T_{\text{boil}}$	739.37	K	Joback Method
$T_c$	1008.22	K	Joback Method
$T_{\text{fus}}$	490.04	K	Joback Method
$V_c$	0.74	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	385.50	J/mol×K	739.37	Joback Method
$\eta$	0.00	Paxs	739.37	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H5Cl5/c13-7-1-6\(2-8\(14\)3-7\)9-4-11\(16\)12\(17\)5-10\(9\)15/h1-5H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H5Cl5/c13-7-1-6(2-8(14)3-7)9-4-11(16)12(17)5-10(9)15/h1-5H)

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

$C_{p, gas}$ : Ideal gas heat capacity (J/molxK).

$\eta$ : Dynamic viscosity (Pa $\times$ s).

$\Delta_f G^\circ$ : Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$ : Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$ : Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$ : Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$ : Octanol/Water partition coefficient .

$P_c$ : Critical Pressure (kPa).

$T_{boil}$ : Normal Boiling Point Temperature (K).

$T_c$ : Critical Temperature (K).

$T_{fus}$ : Normal melting (fusion) point (K).

$V_c$ : Critical Volume (m<sup>3</sup>/kg-mol).

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