

2,2',3,4',6-Pentachloro-1,1'-biphenyl

Other names: 1,1'-Biphenyl, 2,2',3,4',6-pentachloro; PCB 91.

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

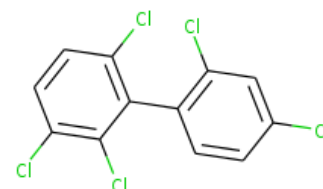
InChI Key: CXKIGWXPPVZSQK-UHFFFAOYSA-N

Formula: C12H5Cl5

SMILES: Clc1ccc(-c2c(Cl)ccc(Cl)c2Cl)c(Cl)c1

Molecular Weight: 326.43

CAS: 68194-05-8



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_{boil}	739.37	K	Joback Method
T_c	1008.22	K	Joback Method
T_{fus}	490.04	K	Joback Method
V_c	0.74	m ³ /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
η	0.00	Paxs	739.37	Joback Method

Sources

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

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

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

Legend

$C_{p, \text{gas}}$: Ideal gas heat capacity (J/mol \times K).

η : Dynamic viscosity (Pa \times s).

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

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

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

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

$\log P_{\text{oct/wat}}$: 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 (m³/kg-mol).

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