1,1'-Biphenyl, 2,2',4,4',5,5'-hexachloro-

Other names: 2,2',4,4',5,5'-Hexachloro-1,1'-biphenyl; 2,2',4,4',5,5'-Hexachlorobiphenyl; 2,4,5,2',4',5'-Hexachlorobiphenyl; Biphenyl, 2,2',4,4',5,5'-hexachloro-; PCB-153.

InChI: InChI=1S/C12H4Cl6/c13-7-3-11(17)9(15)1-5(7)6-2-10(16)12(18)4-8(6)14/h1-4H

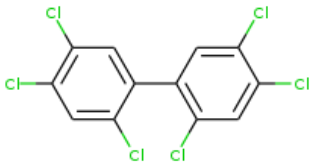
InChI Key: MVWHGTYKUMDIHL-UHFFFAOYSA-N

Formula: C12H4Cl6

SMILES: Clc1cc(Cl)c(-c2cc(Cl)c(Cl)cc2Cl)cc1Cl

Molecular Weight: 360.88

CAS: 35065-27-1



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	145.62	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	18.79	kJ/mol	Joback Method
$\Delta_{fus} H°$	37.77	kJ/mol	Joback Method
$\Delta_{vap} H°$	103.50 ± 0.10	kJ/mol	NIST Webbook
$logP_{oct/wat}$	7.27		Crippen Method
P_c	2450.74	kPa	Joback Method
T_{boil}	781.78	K	Joback Method
T_c	1052.68	K	Joback Method
T_{fus}	532.48	K	Joback Method
V_c	0.79	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	401.07	J/mol×K	781.78	Joback Method
η	0.00	Pa×s	781.78	Joback Method
$\Delta_{vap} H$	91.40	kJ/mol	368.0	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H4Cl6/c13-7-3-11(17)9(15)1-5(7)6-2-10(16)12(18)4-8(6)14/h1-4H
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\Delta_{vap} H$: Enthalpy of vaporization at a given temperature (kJ/mol).
***log*P$_{oct/wat}$**: 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^3/kg-mol).