1,1'-Biphenyl, 2,3',4',5-tetrachloro-

Other names: 2,3',4',5-Tetrachloro-1,1'-biphenyl; 2,3',4',5-Tetrachlorobiphenyl; 2,5,3',4'-Tetrachlorobiphenyl; Biphenyl, 2,3',4',5-tetrachloro-; PCB-70.

InChI: InChI=1S/C12H6Cl4/c13-8-2-4-10(14)9(6-8)7-1-3-11(15)12(16)5-7/h1-6H

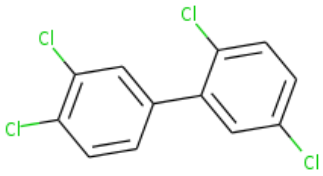
InChI Key: KENZYIHFBRWMOD-UHFFFAOYSA-N

Formula: C12H6Cl4

SMILES: Clc1ccc(Cl)c(-c2ccc(Cl)c(Cl)c2)c1

Molecular Weight: 291.99

CAS: 32598-11-1



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	188.74	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	73.21	kJ/mol	Joback Method
$\Delta_{fus} H°$	30.15	kJ/mol	Joback Method
$\Delta_{vap} H°$	67.05	kJ/mol	Joback Method
$logP_{oct/wat}$	5.97		Crippen Method
P_c	2724.01	kPa	Joback Method
T_{boil}	696.96	K	Joback Method
T_c	963.35	K	Joback Method
T_{fus}	447.60	K	Joback Method
V_c	0.69	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	368.27	J/mol×K	696.96	Joback Method
η	0.00	Pa×s	696.96	Joback Method
$\Delta_{vap} H$	84.80	kJ/mol	370.5	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H6Cl4/c13-8-2-4-10(14)9(6-8)7-1-3-11(15)12(16)5-7/h1-6H
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H}$: Enthalpy of vaporization at a given temperature (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).