

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

Other names: 2,3',5,5'-Tetrachlorobiphenyl; PCB 72.

InChI:

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

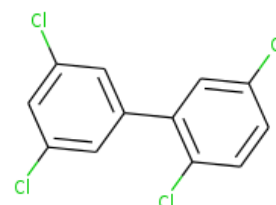
InChI Key: WBTFMEPLVQOWFI-UHFFFAOYSA-N

Formula: C12H6Cl4

SMILES: Clc1ccc(Cl)c(-c2cc(Cl)cc(Cl)c2)c1

Molecular Weight: 291.99

CAS: 41464-42-0



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	188.74	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	73.21	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	30.15	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	67.05	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	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
$C_{p,\text{gas}}$	368.27	J/mol×K	696.96	Joback Method
η	0.00	Paxs	696.96	Joback Method

Sources

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

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H6Cl4/c13-8-1-2-12\(16\)11\(6-8\)7-3-9\(14\)5-10\(15\)4-7/h1-6H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H6Cl4/c13-8-1-2-12(16)11(6-8)7-3-9(14)5-10(15)4-7/h1-6H)

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

Legend

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

η : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$: 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 (m³/kg-mol).

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