1,1'-Biphenyl, 2,3,4,5,6-pentachloro-

Other names: 2,3,4,5,6-Pentachloro-1,1'-biphenyl; 2,3,4,5,6-Pentachlorobiphenyl; Biphenyl, 2,3,4,5,6-pentachloro-; PCB 116.

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

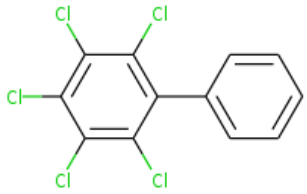
InChI Key: GGMPTLAAIUQMIE-UHFFFAOYSA-N

Formula: C12H5Cl5

SMILES: Clc1c(Cl)c(Cl)c(-c2ccccc2)c(Cl)c1Cl

Molecular Weight: 326.43

CAS: 18259-05-7



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	167.18	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	46.00	kJ/mol	Joback Method
$\Delta_{fus} H°$	33.96	kJ/mol	Joback Method
$\Delta_{vap} H°$	72.09	kJ/mol	Joback Method
$logP_{oct/wat}$	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}	397.60 ± 0.20	K	NIST Webbook
V_c	0.74	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	385.50	J/mol×K	739.37	Joback Method
η	0.00	Pa×s	739.37	Joback Method
$\Delta_{fus} H$	21.80	kJ/mol	397.6	NIST Webbook

Property	Value	Unit	Temperature (K)	Source
$\Delta_{fus}H$	21.80	kJ/mol	397.6	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H5Cl5/c13-8-7(6-4-2-1-3-5-6)9(14)11(16)12(17)10(8)15/h1-5H
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).
Δ_f**G°**: Standard Gibbs free energy of formation (kJ/mol).
Δ_f**H°**$_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{fus}**H**: Enthalpy of fusion at a given temperature (kJ/mol).
Δ_{vap}**H°**: Enthalpy of vaporization at standard conditions (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).