

# Benzene, 1,1'-oxybis[4-chloro-

**Other names:** 4,4'-Dichlorodiphenyl ether; Benzene, 1,1'-oxybis\*4-chloro-; Bis(p-chlorophenyl) ether; Ether, bis(p-chlorophenyl); p,p'-Dichlorodiphenyl oxide.

**InChI:**

InChI=1S/C12H8Cl2O/c13-9-1-5-11(6-2-9)15-12-7-3-10(14)4-8-12/h1-8H

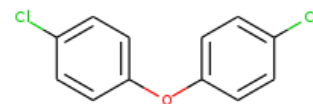
**InChI Key:** URUJZH ZLCC IILC-UHFFFAOYSA-N

**Formula:** C12H8Cl2O

**SMILES:** Clc1ccc(Oc2ccc(Cl)cc2)cc1

**Molecular Weight:** 239.10

**CAS:** 2444-89-5



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	126.86	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-4.59	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	23.72	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	59.36	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.79		Crippen Method
$P_c$	2989.32	kPa	Joback Method
$T_{\text{boil}}$	634.56	K	Joback Method
$T_c$	889.75	K	Joback Method
$T_{\text{fus}}$	384.95	K	Joback Method
$V_c$	0.61	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	351.12	J/mol×K	634.56	Joback Method
$\eta$	0.00	Paxs	634.56	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:**

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H8Cl2O/c13-9-1-5-11\(6-2-9\)15-12-7-3-10\(14\)4-8-12/h1-8H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H8Cl2O/c13-9-1-5-11(6-2-9)15-12-7-3-10(14)4-8-12/h1-8H)

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

## Legend

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

$\eta$ : Dynamic viscosity (Pa×s).

$\Delta_f G^\circ$ : 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 (m<sup>3</sup>/kg-mol).

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