

# Dibenzo-p-dioxin, 1,7-dichloro

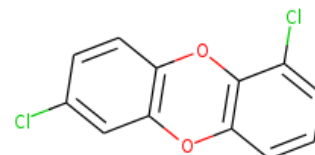
**InChI:** InChI=1S/C12H6Cl2O2/c13-7-4-5-9-11(6-7)15-10-3-1-2-8(14)12(10)16-9/h1-6H

**InChI Key:** IJUWLAFFPPVRYGY-UHFFFAOYSA-N

**Formula:** C12H6Cl2O2

**SMILES:** Clc1ccc2c(c1)Oc1cccc(Cl)c1O2

**Molecular Weight:** 253.08



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	120.92	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-60.01	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	36.88	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	67.35	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.891		Crippen Method
$P_c$	3372.36	kPa	Joback Method
$T_{\text{boil}}$	683.14	K	Joback Method
$T_c$	945.37	K	Joback Method
$T_{\text{fus}}$	466.60	K	Joback Method
$V_c$	0.598	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	357.63	J/mol×K	683.14	Joback Method
$\eta$	0.0005107	Paxs	683.14	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/C12H6Cl2O2/c13-7-4-5-9-11\(6-7\)15-10-3-1-2-8\(14\)12\(10\)16-9/h1-6H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H6Cl2O2/c13-7-4-5-9-11(6-7)15-10-3-1-2-8(14)12(10)16-9/h1-6H)

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

## Legend

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

$\eta$ : Dynamic viscosity (Pa×s).

$\Delta_f G^\circ$ : Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{\text{gas}}$ : Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{fus}} H^\circ$ : Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$ : Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{\text{oct/wat}}$ : Octanol/Water partition coefficient .

$P_c$ : Critical Pressure (kPa).

$T_{\text{boil}}$ : Normal Boiling Point Temperature (K).

$T_c$ : Critical Temperature (K).

$T_{\text{fus}}$ : Normal melting (fusion) point (K).

$V_c$ : Critical Volume (m<sup>3</sup>/kg-mol).

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