

# 1,1,2-trans-5-Tetrachlorocyclohexane

## InChI:

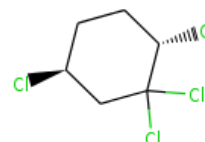
InChI=1S/C6H8Cl4/c7-4-1-2-5(8)6(9,10)3-4/h4-5H,1-3H2/t4-,5-/m1/s1

**InChI Key:** SIJRRCMGPMOBIB-RFZPGFLSSA-N

**Formula:** C<sub>6</sub>H<sub>8</sub>Cl<sub>4</sub>

**SMILES:** ClC1CCC(Cl)C(Cl)(Cl)C1

**Molecular Weight:** 221.94



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-44.54	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-201.25	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	15.76	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	45.15	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.56		Crippen Method
$P_c$	3235.66	kPa	Joback Method
$T_{\text{boil}}$	496.85	K	Joback Method
$T_c$	740.51	K	Joback Method
$T_{\text{fus}}$	299.86	K	Joback Method
$V_c$	0.50	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	246.89	J/mol×K	496.85	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/C6H8Cl4/c7-4-1-2-5\(8\)6\(9,10\)3-4/h4-5H,1-3H2/t4-,5-/m1/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H8Cl4/c7-4-1-2-5(8)6(9,10)3-4/h4-5H,1-3H2/t4-,5-/m1/s1)

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

## Legend

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

$\Delta_f G^\circ$ : 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).

$\log P_{oct/wat}$ : 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<sup>3</sup>/kg-mol).

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