

# 4-Penten-2-ol, trichloroacetate

**InChI:**

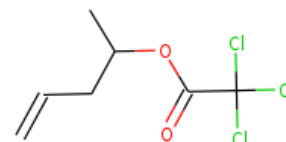
InChI=1S/C7H9Cl3O2/c1-3-4-5(2)12-6(11)7(8,9)10/h3,5H,1,4H2,2H3

**InChI Key:** KCZJXGKHUZQAHL-UHFFFAOYSA-N

**Formula:** C7H9Cl3O2

**SMILES:** C=CCC(C)OC(=O)C(Cl)(Cl)Cl

**Molecular Weight:** 231.50



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-173.41	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-368.43	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	17.05	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	51.13	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.86		Crippen Method
$P_c$	2811.36	kPa	Joback Method
$T_{\text{boil}}$	541.15	K	Joback Method
$T_c$	754.73	K	Joback Method
$T_{\text{fus}}$	316.23	K	Joback Method
$V_c$	0.56	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	300.20	J/mol×K	541.15	Joback Method
$\eta$	0.00	Paxs	541.15	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/C7H9Cl3O2/c1-3-4-5\(2\)12-6\(11\)7\(8,9\)10/h3,5H,1,4H2,2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H9Cl3O2/c1-3-4-5(2)12-6(11)7(8,9)10/h3,5H,1,4H2,2H3)

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

## Legend

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

$\eta$ : Dynamic viscosity (Pa $\times$ 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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