

## (E)-3-Hexen-1-ol, trichloroacetate

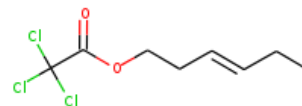
**InChI:** InChI=1S/C8H11Cl3O2/c1-2-3-4-5-6-13-7(12)8(9,10)11/h3-4H,2,5-6H2,1H3/b4-3+

**InChI Key:** HIHSJHFAKCBBNH-ONEGZZNKSA-N

**Formula:** C8H11Cl3O2

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

**Molecular Weight:** 245.53



### Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-170.17	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-392.00	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	24.64	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	54.38	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.26		Crippen Method
$P_c$	2550.76	kPa	Joback Method
$T_{\text{boil}}$	571.95	K	Joback Method
$T_c$	782.40	K	Joback Method
$T_{\text{fus}}$	339.18	K	Joback Method
$V_c$	0.62	m <sup>3</sup> /kg-mol	Joback Method

### Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	343.62	J/mol×K	571.95	Joback Method
$\eta$	0.00	Paxs	571.95	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/C8H11Cl3O2/c1-2-3-4-5-6-13-7\(12\)8\(9,10\)11/h3-4H,2,5-6H2,1H3/b4-3+](http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H11Cl3O2/c1-2-3-4-5-6-13-7(12)8(9,10)11/h3-4H,2,5-6H2,1H3/b4-3+)

**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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