

4-Penten-2-ol, chloroacetate

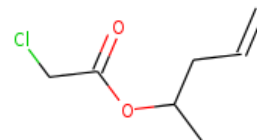
InChI: InChI=1S/C7H11ClO2/c1-3-4-6(2)10-7(9)5-8/h3,6H,1,4-5H2,2H3

InChI Key: MLUZZPKUPKESMI-UHFFFAOYSA-N

Formula: C7H11ClO2

SMILES: C=CCC(C)OC(=O)CCl

Molecular Weight: 162.61



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-152.39	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-328.20	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	16.07	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	43.66	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.73		Crippen Method
P_c	2982.79	kPa	Joback Method
T_{boil}	469.52	K	Joback Method
T_c	660.02	K	Joback Method
T_{fus}	253.97	K	Joback Method
V_c	0.48	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	248.56	J/mol×K	469.52	Joback Method
η	0.00	Paxs	469.52	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H11ClO2/c1-3-4-6\(2\)10-7\(9\)5-8/h3,6H,1,4-5H2,2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H11ClO2/c1-3-4-6(2)10-7(9)5-8/h3,6H,1,4-5H2,2H3)

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

Legend

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

η : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$: 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 (m³/kg-mol).

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