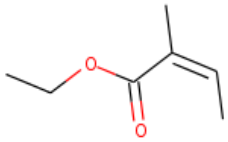
(Z)-Ethyl 2-methylbut-2-enoate

InChI: InChI=1S/C7H12O2/c1-4-6(3)7(8)9-5-2/h4H,5H2,1-3H3/b6-4-
InChI Key: OAPHLAAOJMTMLY-XQRVVYSFSA-N
Formula: C7H12O2
SMILES: CC=C(C)C(=O)OCC
Molecular Weight: 128.17
CAS: 16509-44-7



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-154.19	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-325.18	kJ/mol	Joback Method
$\Delta_{fus} H°$	15.56	kJ/mol	Joback Method
$\Delta_{vap} H°$	40.37	kJ/mol	Joback Method
$logP_{oct/wat}$	1.52		Crippen Method
P_c	3131.49	kPa	Joback Method
T_{boil}	439.89	K	Joback Method
T_c	628.49	K	Joback Method
T_{fus}	221.77	K	Joback Method
V_c	0.43	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	222.62	J/mol×K	439.89	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H12O2/c1-4-6(3)7(8)9-5-2/h4H,5H2,1-3H3/b6-4-
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).