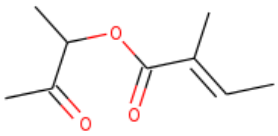
3-Oxobutan-2-yl (E)-2-methylbut-2-enoate

InChI:
InChI=1S/C9H14O3/c1-5-6(2)9(11)12-8(4)7(3)10/h5,8H,1-4H3/b6-5+
InChI Key: PNUCZORMJRDQRQ-AATRIKPKSA-N
Formula: C9H14O3
SMILES: CC=C(C)C(=O)OC(C)C(C)=O
Molecular Weight: 170.21



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-268.71	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-484.32	kJ/mol	Joback Method
$\Delta_{fus} H°$	18.82	kJ/mol	Joback Method
$\Delta_{vap} H°$	51.18	kJ/mol	Joback Method
$logP_{oct/wat}$	1.473		Crippen Method
P_c	2746.90	kPa	Joback Method
T_{boil}	539.08	K	Joback Method
T_c	737.09	K	Joback Method
T_{fus}	279.24	K	Joback Method
V_c	0.544	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	325.07	J/mol×K	539.08	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H14O3/c1-5-6(2)9(11)12-8(4)7(3)10/h5,8H,1-4H3/b6-5+
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: 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^3/kg-mol).