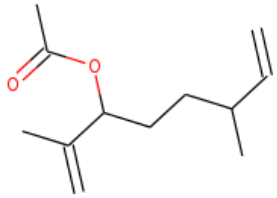
2,6-Dimethyl-1,7-octadien-3-ol, acetate

Other names: 1-isopropenyl-4-methylhex-5-enyl acetate.
InChI: InChI=1S/C12H20O2/c1-6-10(4)7-8-12(9(2)3)14-11(5)13/h6,10,12H,1-2,7-8H2,3-5H3
InChI Key: ATOCHKMVAHBPNF-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: C=CC(C)CCC(OC(C)=O)C(=C)C
Molecular Weight: 196.29
CAS: 61382-99-8



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-21.51	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-305.30	kJ/mol	Joback Method
$\Delta_{fus} H°$	18.71	kJ/mol	Joback Method
$\Delta_{vap} H°$	49.43	kJ/mol	Joback Method
$logP_{oct/wat}$	3.10		Crippen Method
P_c	2030.89	kPa	Joback Method
T_{boil}	542.61	K	Joback Method
T_c	728.14	K	Joback Method
T_{fus}	249.68	K	Joback Method
V_c	0.68	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	425.09	J/mol×K	542.61	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H20O2/c1-6-10(4)7-8-12(9(2)3)14-11(5)13/h6,10,12H,1-2,7-8H2,3-5H3

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).