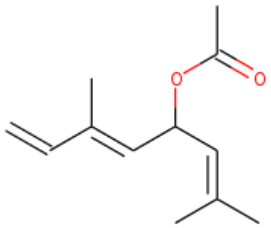
(E)-Ocimenyl acetate

InChI: InChI=1S/C12H18O2/c1-6-10(4)8-12(7-9(2)3)14-11(5)13/h6-8,12H,1H2,2-5H3/b10-8+
InChI Key: ZOOSZTPUIIHGKF-CSKARUKUSA-N
Formula: C12H18O2
SMILES: C=CC(C)=CC(C=C(C)C)OC(C)=O
Molecular Weight: 194.27



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	44.98	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-200.80	kJ/mol	Joback Method
$\Delta_{fus} H°$	22.60	kJ/mol	Joback Method
$\Delta_{vap} H°$	50.48	kJ/mol	Joback Method
$logP_{oct/wat}$	3.02		Crippen Method
P_c	2143.35	kPa	Joback Method
T_{boil}	554.57	K	Joback Method
T_c	751.89	K	Joback Method
T_{fus}	242.32	K	Joback Method
V_c	0.67	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	407.13	J/mol×K	554.57	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H18O2/c1-6-10(4)8-12(7-9(2)3)14-11(5)13/h6-8,12H,1H2,2-5H3/b10-8+

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).

Latest version available from:
https://old.chemeo.com/cid/85-688-5/%28E%29-Ocimenyl%20acetate
Generated by Cheméo on Wed, 26 Jan 2022 23:13:13 +0000.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.