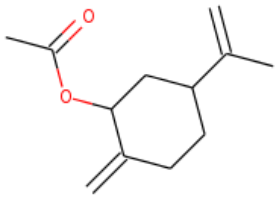
p-mentha-1(7),8-dien-2-yl acetate

Other names: menthadien-2-yl acetate, p-1(7),8.
InChI: InChI=1S/C12H18O2/c1-8(2)11-6-5-9(3)12(7-11)14-10(4)13/h11-12H,1,3,5-7H2,2,4H3
InChI Key: CCLNPVCMIJDJLR-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: C=C(C)C1CCC(=C)C(OC(C)=O)C1
Molecular Weight: 194.27
CAS: 1134-96-9



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-34.65	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-301.95	kJ/mol	Joback Method
$\Delta_{fus} H°$	18.78	kJ/mol	Joback Method
$\Delta_{vap} H°$	51.15	kJ/mol	Joback Method
$logP_{oct/wat}$	2.85		Crippen Method
P_c	2298.11	kPa	Joback Method
T_{boil}	560.85	K	Joback Method
T_c	769.45	K	Joback Method
T_{fus}	298.26	K	Joback Method
V_c	0.63	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	414.55	J/mol×K	560.85	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H18O2/c1-8(2)11-6-5-9(3)12(7-11)14-10(4)13/h11-12H,1,3,5-7H2,2,4H3

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: 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).