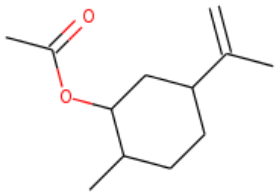
Neoiso-dihydrocarveol acetate

InChI: InChI=1S/C12H20O2/c1-8(2)11-6-5-9(3)12(7-11)14-10(4)13/h9,11-12H,1,5-7H2,2-4H3
InChI Key: TUSIZTVSUSBSQI-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: C=C(C)C1CCC(C)C(OC(C)=O)C1
Molecular Weight: 196.29



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-95.44	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-406.53	kJ/mol	Joback Method
$\Delta_{fus} H°$	21.01	kJ/mol	Joback Method
$\Delta_{vap} H°$	50.68	kJ/mol	Joback Method
$logP_{oct/wat}$	2.930		Crippen Method
P_c	2187.68	kPa	Joback Method
T_{boil}	557.02	K	Joback Method
T_c	763.76	K	Joback Method
T_{fus}	280.34	K	Joback Method
V_c	0.644	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	435.53	J/mol×K	557.02	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H20O2/c1-8(2)11-6-5-9(3)12(7-11)14-10(4)13/h9,11-12H,1,5-7H2,2-4H3

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: 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).

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