Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate, (1«alpha»,2«beta»,5«beta»)-

Other names: Isomenthol acetate; Isomenthyl acetate; Menthol, acetate, iso-.

InChI: InChI=1S/C12H22O2/c1-8(2)11-6-5-9(3)7-12(11)14-10(4)13/h8-9,11-12H,5-7H2,1-4H3/t9-,11-,12+/m0/s1

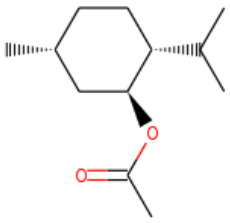
InChI Key: XHXUANMFYXWVNG-ZMLRMANQSA-N

Formula: C12H22O2

SMILES: CC(=O)OC1CC(C)CCC1C(C)C

Molecular Weight: 198.30

CAS: 20777-45-1



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-177.17	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-527.45	kJ/mol	Joback Method
$\Delta_{fus} H°$	20.08	kJ/mol	Joback Method
$\Delta_{vap} H°$	50.89	kJ/mol	Joback Method
$logP_{oct/wat}$	3.010		Crippen Method
P_c	2110.00	kPa	Joback Method
T_{boil}	560.02	K	Joback Method
T_c	763.29	K	Joback Method
T_{fus}	281.06	K	Joback Method
V_c	0.656	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	456.30	J/mol×K	560.02	Joback Method
η	0.0002377	Pa×s	560.02	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H22O2/c1-8(2)11-6-5-9(3)7-12(11)14-10(4)13/h8-9,11-12H,5-7H2,1-4H3/t9-,11-,12+/m0/s1
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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