

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

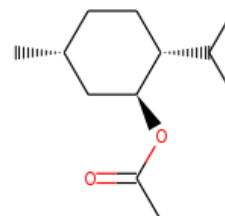
InChI Key: XHXUANMFYXWVNG-ZMLRMANQSA-N

Formula: C₁₂H₂₂O₂

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

Molecular Weight: 198.30

CAS: 20777-45-1



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-177.17	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-527.45	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	20.08	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	50.89	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	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
$C_{p,\text{gas}}$	456.30	J/mol×K	560.02	Joback Method
η	0.0002377	Paxs	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](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/ci9903071>

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).

η : Dynamic viscosity (Pa×s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

Latest version available from:

<https://old.cheméo.com/cid/11-804-6/Cyclohexanol%2C%205-methyl-2-%281-methylethyl%29-%2C%20acetate%2C%20%281%2C%20ABalpha%2C%20BB%2C%20ABbeta%2C%20BB%2C5%2C%20ABbeta%2C%20BB%29->

Generated by Cheméo on Tue, 16 Aug 2022 04:46:35 +0000.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.