

isopulegol acetate

Other names: Isopulegol acetate (Isomer 2); isopulegol acetate (isomer 1).

InChI: InChI=1S/C12H20O2/c1-8(2)11-6-5-9(3)7-12(11)14-10(4)13/h9,11-12H,1,5-7H2,2-4H3/t9-,11+,12-/m1/s1

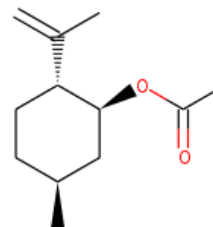
InChI Key: HLHIVJRL0DSUCI-ADEWGFFLSA-N

Formula: C₁₂H₂₀O₂

SMILES: C=C(C)C1CCC(C)CC1OC(C)=O

Molecular Weight: 196.29

CAS: 109010-12-0



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-95.44	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-406.53	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	21.01	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	50.68	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	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
$C_{p,\text{gas}}$	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\(3\)7-12\(11\)14-10\(4\)13/h9,11-12H,1,5-7H2,2-4H3/t9-,11+,12-/m1/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H20O2/c1-8(2)11-6-5-9(3)7-12(11)14-10(4)13/h9,11-12H,1,5-7H2,2-4H3/t9-,11+,12-/m1/s1)

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

Legend

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

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

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

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

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

$\log P_{\text{oct/wat}}$: 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).

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