

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

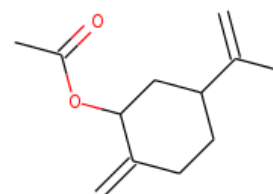
InChI Key: CCLNPVCMIJDLR-UHFFFAOYSA-N

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
$\Delta_f G^\circ$	-34.65	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-301.95	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	18.78	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	51.15	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	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
$C_{p,\text{gas}}$	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](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/ci9903071>

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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