

# Fragranyl acetate

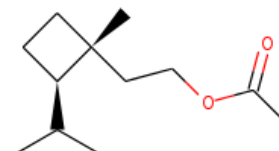
**InChI:** InChI=1S/C12H22O2/c1-9(2)11-5-6-12(11,4)7-8-14-10(3)13/h9,11  
H,5-8H2,1-4H3/t11-,12-/m1/s1

**InChI Key:** WHLCYZCJPXWYQN-VXGBXAGGSA-N

**Formula:** C<sub>12</sub>H<sub>22</sub>O<sub>2</sub>

**SMILES:** CC(=O)OCCC1(C)CCC1C(C)C

**Molecular Weight:** 198.30



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-150.75	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-479.55	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	16.91	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	49.70	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.01		Crippen Method
$P_c$	2165.35	kPa	Joback Method
$T_{\text{boil}}$	556.39	K	Joback Method
$T_c$	753.90	K	Joback Method
$T_{\text{fus}}$	316.24	K	Joback Method
$V_c$	0.67	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	451.93	J/mol×K	556.39	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H22O2/c1-9\(2\)11-5-6-12\(11,4\)7-8-14-10\(3\)13/h9,11H,5-8H2,1-4H3/t11-,12-/m1/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H22O2/c1-9(2)11-5-6-12(11,4)7-8-14-10(3)13/h9,11H,5-8H2,1-4H3/t11-,12-/m1/s1)

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

## Legend

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

$\Delta_f G^\circ$ : 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).

$\log P_{oct/wat}$ : 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 (m<sup>3</sup>/kg-mol).

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