

.beta.-Isocyclolavandulyl acetate

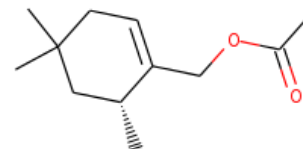
InChI: InChI=1S/C12H20O2/c1-9-7-12(3,4)6-5-11(9)8-14-10(2)13/h5,9H,6-8H2,1-4H3/t9-/m0/s1

InChI Key: QHJKSPVTMXZZCA-VIFPVBQESA-N

Formula: C12H20O2

SMILES: CC(=O)OCC1=CCC(C)(C)CC1C

Molecular Weight: 196.29



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-152.18	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-440.28	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	17.06	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	51.39	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.932		Crippen Method
P_c	2298.11	kPa	Joback Method
T_{boil}	569.51	K	Joback Method
T_c	779.44	K	Joback Method
T_{fus}	337.48	K	Joback Method
V_c	0.647	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	434.86	J/mol×K	569.51	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H20O2/c1-9-7-12\(3,4\)6-5-11\(9\)8-14-10\(2\)13/h5,9H,6-8H2,1-4H3/t9-/m0/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H20O2/c1-9-7-12(3,4)6-5-11(9)8-14-10(2)13/h5,9H,6-8H2,1-4H3/t9-/m0/s1)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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 (m³/kg-mol).

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