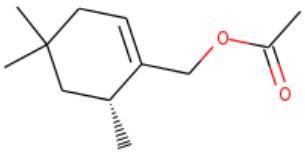
.beta.-Isocyclolavandulyl acetate

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
$\Delta_f G°$	-152.18	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-440.28	kJ/mol	Joback Method
$\Delta_{fus} H°$	17.06	kJ/mol	Joback Method
$\Delta_{vap} H°$	51.39	kJ/mol	Joback Method
$logP_{oct/wat}$	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
$C_{p,gas}$	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

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

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: 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^3/kg-mol).