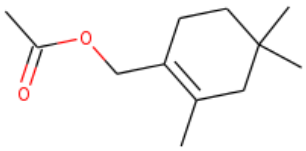
«beta»-Cyclolavandulyl acetate

InChI:
InChI=1S/C12H20O2/c1-9-7-12(3,4)6-5-11(9)8-14-10(2)13/h5-8H2,1-4H3
InChI Key: PJBZKRBNXOKTOE-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: CC(=O)OCC1=C(C)CC(C)(C)CC1
Molecular Weight: 196.29



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-154.10	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-431.41	kJ/mol	Joback Method
$\Delta_{fus} H°$	15.60	kJ/mol	Joback Method
$\Delta_{vap} H°$	52.36	kJ/mol	Joback Method
$logP_{oct/wat}$	3.08		Crippen Method
P_c	2338.29	kPa	Joback Method
T_{boil}	579.16	K	Joback Method
T_c	790.19	K	Joback Method
T_{fus}	354.24	K	Joback Method
V_c	0.65	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	433.72	J/mol×K	579.16	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/h5-8H2,1-4H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).