24-Ethyl-25-dehydrolophenol acetate, 24-.beta.

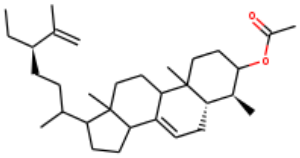
InChI: InChI=1S/C32H52O2/c1-9-24(20(2)3)11-10-21(4)26-14-15-28-25-12-13-27-22(5)30(34-23(6)33)17-19-32(27,8)29(25)16-18-31(26,28)7/h12,21-22,24,26-30H,2,9-11,13-19H2,1,3-8H3/t21?,22-,24+,26?,27-,28?,29?,30?,31?,32?/m1/s1

InChI Key: UACMKUJYWHZEHR-GBSVDFTQSA-N

Formula: C32H52O2

SMILES: C=C(C)C(CC)CCC(C)C1CCC2C3=CCC4C(C)C(OC(C)=O)CCC4(C)C3CCC21C

Molecular Weight: 468.75



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	220.06	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-587.70	kJ/mol	Joback Method
$\Delta_{fus} H°$	46.35	kJ/mol	Joback Method
$\Delta_{vap} H°$	92.54	kJ/mol	Joback Method
$log P_{oct/wat}$	8.76		Crippen Method
P_c	790.37	kPa	Joback Method
T_{boil}	1037.78	K	Joback Method
T_c	1273.34	K	Joback Method
T_{fus}	575.12	K	Joback Method
V_c	1.59	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1619.08	J/mol×K	1037.78	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C32H52O2/c1-9-24(20(2)3)11-10-21(4)26-14-15-28-25-12-13-27-22(5)30(34-23(6)33)17-19-32(27,8)29(25)16-18-31(26,28)7/h12,21-22,24,26-30H,2,9-11,13-19H2,1,3-8H3/t21?,22-,24+,26?,27-,28?,29?,30?,31?,32?/m1/s1

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

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: 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).
$logP_{oct/wat}$: 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).