24-Methylene-24-dihydrolanosterol acetate

InChI: InChI=1S/C33H54O2/c1-21(2)22(3)11-12-23(4)25-15-19-33(10)27-13-14-28-30(6,7)29(35-24(5)34)17-18-31(28,8)26(27)16-20-32(25,33)9/h21,23,25,28-29H,3,11-20H2,1-2,4-10H3

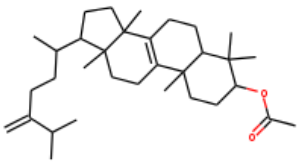
InChI Key: XJAUCFFDVQSSEW-UHFFFAOYSA-N

Formula: C33H54O2

SMILES: C=C(CCC(C)C1CCC2(C)C3=C(CCC12C)C1(C)CCC(OC(C)=O)C(C)(C)C1CC3)C(C)C

Molecular Weight: 482.78

CAS: 17837-80-8



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	215.58	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-568.99	kJ/mol	Joback Method
$\Delta_{fus} H°$	34.88	kJ/mol	Joback Method
$\Delta_{vap} H°$	93.44	kJ/mol	Joback Method
$logP_{oct/wat}$	9.30		Crippen Method
P_c	795.73	kPa	Joback Method
T_{boil}	1070.79	K	Joback Method
T_c	1314.23	K	Joback Method
T_{fus}	650.95	K	Joback Method
V_c	1.64	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1728.47	J/mol×K	1070.79	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C33H54O2/c1-21(2)22(3)11-12-23(4)25-15-19-33(10)27-13-14-28-30(6,7)29(35-24(5)34)17-18-31(28,8)26(27)16-20-32(25,33)9/h21,23,25,28-29H,3,11-20H2,1-2,4-10H3

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).