Vernosterol acetate

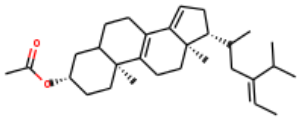
InChI: InChI=1S/C30H46O2/c1-8-22(19(2)3)17-20(4)26-11-12-27-25-10-9-23-18-24(32-21(5)31)13-15-29(23,6)28(25)14-16-30(26,27)7/h8,12,19-20,23-24,26H,9-11,13-18H2,1-7H3/b22-8-/t20?,23?,24-,26+,29-,30+/m1/s1

InChI Key: ORZLNKKIYBRHAR-ZMFSMEMUSA-N

Formula: C30H46O2

SMILES: CC=C(CC(C)C1CC=C2C3=C(CCC21C)C1(C)CCC(OC(C)=O)CC1CC3)C(C)C

Molecular Weight: 438.68



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	229.43	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-458.77	kJ/mol	Joback Method
$\Delta_{fus} H°$	39.88	kJ/mol	Joback Method
$\Delta_{vap} H°$	91.26	kJ/mol	Joback Method
$logP_{oct/wat}$	8.19		Crippen Method
P_c	946.75	kPa	Joback Method
T_{boil}	1022.63	K	Joback Method
T_c	1261.04	K	Joback Method
T_{fus}	587.78	K	Joback Method
V_c	1.46	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1441.58	J/mol×K	1022.63	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C30H46O2/c1-8-22(19(2)3)17-20(4)26-11-12-27-25-10-9-23-18-24(32-21(5)31)13-15-29(23,6)28(25)14-16-30(26,27)7/h8,12,19-20,23-24,26H,9-11,13-18H2,1-7H3/b22-8-/t20?,23?,24-,26+,29-,30+/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).
***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).