Tirucallol acetate

InChI: InChI=1S/C32H52O2/c1-21(2)11-10-12-22(3)24-15-19-32(9)26-13-14-27-29(5,6)28(34-23(4)33)17-18-30(27,7)25(26)16-20-31(24,32)8/h11,22,24,27-28H,10,12-20H2,1-9H3/t22-,24-,27?,28-,30+,31-,32+/m1/s1

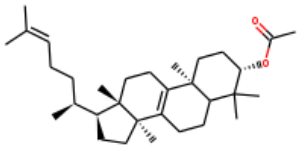
InChI Key: BQPPJGMMIYJVBR-NUBGRVATSA-N

Formula: C32H52O2

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

Molecular Weight: 468.75

CAS: 52689-37-9



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	201.98	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-551.28	kJ/mol	Joback Method
$\Delta_{fus} H°$	37.30	kJ/mol	Joback Method
$\Delta_{vap} H°$	92.23	kJ/mol	Joback Method
$logP_{oct/wat}$	9.05		Crippen Method
P_c	841.62	kPa	Joback Method
T_{boil}	1055.83	K	Joback Method
T_c	1298.35	K	Joback Method
T_{fus}	651.36	K	Joback Method
V_c	1.59	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1654.54	J/mol×K	1055.83	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C32H52O2/c1-21(2)11-10-12-22(3)24-15-19-32(9)26-13-14-27-29(5,6)28(34-23(4)33)17-18-30(27,7)25(26)16-20-31(24,32)8/h11,22,24,27-28H,10,12-20H2,1-9H3/t22-,24-,27?,28-,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).
***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).