

5.alpha.-tirucalla-8,23-dien-3.beta.-ol, acetylated

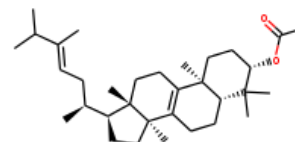
InChI: InChI=1S/C33H54O2/c1-21(2)22(3)11-12-23(4)25-15-19-33(10)27-13-14-28-30(6,7)29(35-24(5)34)17-18-31(28,8)26(27)16-20-32(25,33)9/h1,21,23,25,28-29H,12-20H2,1-10H3/b22-11+/t23-,25-,28-,29-,31+,32-,33+/m1/s1

InChI Key: DJFUFRXAOIPMAV-LRQVTKJASA-N

Formula: C₃₃H₅₄O₂

SMILES: CC(=O)OC1CCC2(C)C3=C(CCC2C1(C)C)C1(C)CCC(C(C)CC=C(C)C(C)C)C1(C)CC3

Molecular Weight: 482.78



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	207.96	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-577.20	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	36.36	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	94.07	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	9.30		Crippen Method
P_c	800.24	kPa	Joback Method
T_{boil}	1078.27	K	Joback Method
T_c	1323.90	K	Joback Method
T_{fus}	647.63	K	Joback Method
V_c	1.64	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1737.04	J/mol×K	1078.27	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/h11,21,23,25,28-29H,12-20H2,1-10H3/b22-11+/t23-,25-,28-,29-,31+,32-,33+/m1/s1](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/h11,21,23,25,28-29H,12-20H2,1-10H3/b22-11+/t23-,25-,28-,29-,31+,32-,33+/m1/s1)

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

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: 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 (m³/kg-mol).

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