

8(15)-Cedren-9-«alpha»-ol, acetate

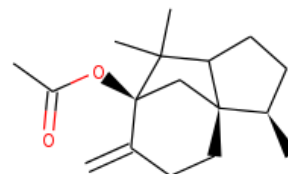
InChI: InChI=1S/C17H26O2/c1-11-6-7-14-15(4,5)17(19-13(3)18)10-16(11,14)9-8-12(17)2/h11,14H,2,6-10H2,1,3-5H3/t11-,14?,16+,17-/m0/s1

InChI Key: YFYJISUDJNNDIJ-MDMQDRFWSA-N

Formula: C17H26O2

SMILES: C=C1CCC23CC1(OC(C)=O)C(C)(C)C2CCC3C

Molecular Weight: 262.39



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	37.58	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-343.65	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	14.87	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	58.76	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.10		Crippen Method
P_c	1930.44	kPa	Joback Method
T_{boil}	683.95	K	Joback Method
T_c	912.08	K	Joback Method
T_{fus}	477.19	K	Joback Method
V_c	0.84	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	663.97	J/mol×K	683.95	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H26O2/c1-11-6-7-14-15\(4,5\)17\(19-13\(3\)18\)10-16\(11,14\)9-8-12\(17\)2/h11,14H,2,6-10H2,1,3-5H3/t11-,14?,16+,17-/m0/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H26O2/c1-11-6-7-14-15(4,5)17(19-13(3)18)10-16(11,14)9-8-12(17)2/h11,14H,2,6-10H2,1,3-5H3/t11-,14?,16+,17-/m0/s1)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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