

(E)-Opposita-4(15),7(11)-dien-12-ol

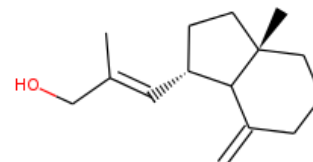
InChI: InChI=1S/C15H24O/c1-11(10-16)9-13-6-8-15(3)7-4-5-12(2)14(13)15/h9,13-14,16H,2,4-8,10H2,1,3H3/b11-9+/t13-,14?,15-/m1/s1

InChI Key: AYGQNVSBUDGKN-BJRRHPIXSA-N

Formula: C₁₅H₂₄O

SMILES: C=C1CCCC2(C)CCC(C=C(C)CO)C12

Molecular Weight: 220.35



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	135.35	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-191.47	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	21.17	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	64.74	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.70		Crippen Method
P_c	2177.49	kPa	Joback Method
T_{boil}	659.84	K	Joback Method
T_c	865.08	K	Joback Method
T_{fus}	359.25	K	Joback Method
V_c	0.75	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	570.29	J/mol×K	659.84	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H24O/c1-11\(10-16\)9-13-6-8-15\(3\)7-4-5-12\(2\)14\(13\)15/h9,13-14,16H,2,4-8,10H2,1,3H3/b11-9+/t13-,14?,15-/m1/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H24O/c1-11(10-16)9-13-6-8-15(3)7-4-5-12(2)14(13)15/h9,13-14,16H,2,4-8,10H2,1,3H3/b11-9+/t13-,14?,15-/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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