

Aristolochene

InChI: InChI=1S/C15H24/c1-11(2)13-8-9-14-7-5-6-12(3)15(14,4)10-13/h9,12-13H,1,5-8,10H2,2-4H3

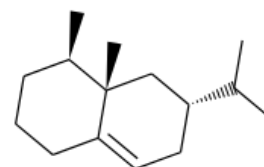
InChI Key: YONHOSLUBQJXPR-UHFFFAOYSA-N

Formula: C15H24

SMILES: CC(C)C1CC=C2CCCC(C)C2(C)C1

Molecular Weight: 204.35

CAS: 26620-71-3



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	153.21	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-196.04	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	14.56	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	48.60	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.805		Crippen Method
P_c	1963.07	kPa	Joback Method
T_{boil}	572.43	K	Joback Method
T_c	793.31	K	Joback Method
T_{fus}	298.55	K	Joback Method
V_c	0.735	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	521.00	J/mol×K	572.43	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H24/c1-11\(2\)13-8-9-14-7-5-6-12\(3\)15\(14,4\)10-13/h9,12-13H,1,5-8,10H2,2-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H24/c1-11(2)13-8-9-14-7-5-6-12(3)15(14,4)10-13/h9,12-13H,1,5-8,10H2,2-4H3)

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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