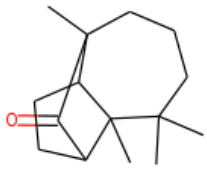
Longicamphenylene

Other names: Longicamphenylone.
InChI: InChI=1S/C15H24O/c1-13(2)8-5-9-14(3)11-7-6-10(12(14)16)15(11,13)4/h10-11H,5-9H2,1-4H3
InChI Key: VMYWIJUHQAMXNC-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC12CCCC(C)(C)C3(C)C(CCC13)C2=O
Molecular Weight: 220.35



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	78.99	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-279.51	kJ/mol	Joback Method
$\Delta_{fus} H°$	7.57	kJ/mol	Joback Method
$\Delta_{vap} H°$	49.24	kJ/mol	Joback Method
$logP_{oct/wat}$	3.82		Crippen Method
P_c	2237.64	kPa	Joback Method
T_{boil}	630.56	K	Joback Method
T_c	875.45	K	Joback Method
T_{fus}	437.03	K	Joback Method
V_c	0.73	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	561.94	J/mol×K	630.56	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H24O/c1-13(2)8-5-9-14(3)11-7-6-10(12(14)16)15(11,13)4/h10-11H,5-9H2,1-4H3

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).