

(E)-3-Butylidene-4,5-dihydroisobenzofuran-1(3H)-one

Other names: (E)-Ligustilide; 1(3H)-Isobenzofuranone, 3-butylidene-4,5-dihydro-, (3E)-; trans-3-Butylidene-4,5-dihydrophthalide; trans-Ligustilide.

InChI: InChI=1S/C12H14O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h5,7-8H,2-4,6H2,1H3/b11-8+

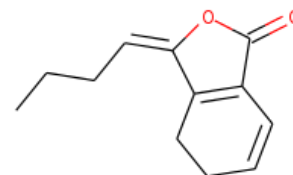
InChI Key: IQVQXVFMNOFTMU-DHZHZOJOSA-N

Formula: C₁₂H₁₄O₂

SMILES: CCCC=C1OC(=O)C2=CC=CC=C12

Molecular Weight: 190.24

CAS: 81944-08-3



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	28.19	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-224.26	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	24.14	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	54.72	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.87		Crippen Method
P_c	2853.57	kPa	Joback Method
T_{boil}	619.28	K	Joback Method
T_c	852.20	K	Joback Method
T_{fus}	390.51	K	Joback Method
V_c	0.58	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	391.29	J/mol×K	619.28	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H14O2/c1-2-3-8-11-9-6-4-5-7-10\(9\)12\(13\)14-11/h5,7-8H,2-4,6H2,1H3/b11-8+](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H14O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h5,7-8H,2-4,6H2,1H3/b11-8+)

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).

$logP_{oct/wat}$: 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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