

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

**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-

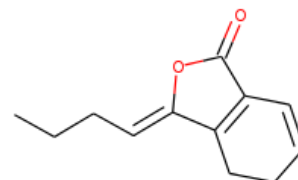
**InChI Key:** IQVQXVFMNOFTMU-FLIBITNWSA-N

**Formula:** C12H14O2

**SMILES:** CCCC=C1OC(=O)C2=C1CCC=C2

**Molecular Weight:** 190.24

**CAS:** 81944-09-4



## 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
$T_{\text{boil}}$	619.28	K	Joback Method
$T_c$	852.20	K	Joback Method
$T_{\text{fus}}$	390.51	K	Joback Method
$V_c$	0.58	m <sup>3</sup> /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](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 (m<sup>3</sup>/kg-mol).

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