

# Cyclobutanecarboxylic acid, hex-4-yn-3-yl ester

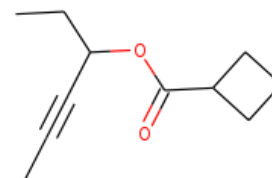
**InChI:** InChI=1S/C11H16O2/c1-3-6-10(4-2)13-11(12)9-7-5-8-9/h9-10H,4-5,7-8H2,1-2H3

**InChI Key:** YQYKIUIBLHLILR-UHFFFAOYSA-N

**Formula:** C11H16O2

**SMILES:** CC#CC(CC)OC(=O)C1CCC1

**Molecular Weight:** 180.24



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	56.83	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-181.51	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	22.67	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	51.08	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.13		Crippen Method
$P_c$	2755.56	kPa	Joback Method
$T_{\text{boil}}$	546.94	K	Joback Method
$T_c$	764.22	K	Joback Method
$T_{\text{fus}}$	391.41	K	Joback Method
$V_c$	0.58	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	367.11	J/mol×K	546.94	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/C11H16O2/c1-3-6-10\(4-2\)13-11\(12\)9-7-5-8-9/h9-10H,4-5,7-8H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H16O2/c1-3-6-10(4-2)13-11(12)9-7-5-8-9/h9-10H,4-5,7-8H2,1-2H3)

**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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