

# 1,3-Cyclohexanedione, 4-propyl-

**InChI:** InChI=1S/C9H14O2/c1-2-3-7-4-5-8(10)6-9(7)11/h7H,2-6H2,1H3

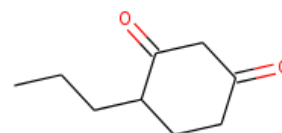
**InChI Key:** WWLVJBISOZBFCG-UHFFFAOYSA-N

**Formula:** C<sub>9</sub>H<sub>14</sub>O<sub>2</sub>

**SMILES:** CCCC1CCC(=O)CC1=O

**Molecular Weight:** 154.21

**CAS:** 18456-81-0



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-195.83	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-450.17	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	9.92	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	44.55	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.725		Crippen Method
$P_c$	3062.55	kPa	Joback Method
$T_{\text{boil}}$	560.51	K	Joback Method
$T_c$	792.97	K	Joback Method
$T_{\text{fus}}$	335.01	K	Joback Method
$V_c$	0.486	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	323.42	J/mol×K	560.51	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/C9H14O2/c1-2-3-7-4-5-8\(10\)6-9\(7\)11/h7H,2-6H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H14O2/c1-2-3-7-4-5-8(10)6-9(7)11/h7H,2-6H2,1H3)

**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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