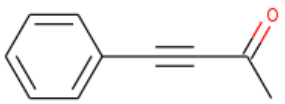
# 4-Phenyl-3-butyn-2-one

**Other names**: 1-Phenyl-1-butyn-3-one; 3-Butyn-2-one, 4-phenyl-; 4-phenylbut-3-yn-2-one.
**InChI**: InChI=1S/C10H8O/c1-9(11)7-8-10-5-3-2-4-6-10/h2-6H,1H3
**InChI Key**: UPEUQDJSUFHFQP-UHFFFAOYSA-N
**Formula**: C10H8O
**SMILES**: CC(=O)C#Cc1ccccc1
**Molecular Weight**: 144.17
**CAS**: 1817-57-8




## Physical Properties

| Property | Value | Unit | Source |
|---|---|---|---|
| $\Delta_c H°_{liquid}$ | -5173.10 | kJ/mol | NIST Webbook |
| $\Delta_f G°$ | 219.61 | kJ/mol | Joback Method |
| $\Delta_f H°_{gas}$ | 146.52 | kJ/mol | Joback Method |
| $\Delta_f H°_{liquid}$ | 94.70 ± 5.00 | kJ/mol | NIST Webbook |
| $\Delta_f H°_{liquid}$ | -63.60 | kJ/mol | NIST Webbook |
| $\Delta_{fus} H°$ | 20.42 | kJ/mol | Joback Method |
| $\Delta_{vap} H°$ | 49.03 | kJ/mol | Joback Method |
| $logP_{oct/wat}$ | 1.627 | | Crippen Method |
| $P_c$ | 3791.65 | kPa | Joback Method |
| $T_{boil}$ | 351.50 ± 0.50 | K | NIST Webbook |
| $T_{boil}$ | 348.70 | K | NIST Webbook |
| $T_c$ | 762.42 | K | Joback Method |
| $T_{fus}$ | 384.91 | K | Joback Method |
| $V_c$ | 0.456 | $m^3$/kg-mol | Joback Method |

## Temperature Dependent Properties

| Property | Value | Unit | Temperature (K) | Source |
|---|---|---|---|---|
| $C_{p,gas}$ | 241.97 | J/mol×K | 517.75 | Joback Method |

## Sources

**Joback Method**: https://en.wikipedia.org/wiki/Joback_method
**NIST Webbook**: http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H8O/c1-9(11)7-8-10-5-3-2-4-6-10/h2-6H,1H3
**Crippen Method**: http://pubs.acs.org/doi/abs/10.1021/ci990307l

## Legend

$\Delta_c H°_{liquid}$: Standard liquid enthalpy of combustion (kJ/mol).
$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_f H°_{liquid}$: Liquid phase enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: 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 ($m^3$/kg-mol).