1-Butanone, 1-phenyl-

Other names: 1-Phenyl-1-butanone; Butyrophenone; Phenyl propyl ketone; Propyl phenyl ketone; n-Butyrophenone.

InChI: InChI=1S/C10H12O/c1-2-6-10(11)9-7-4-3-5-8-9/h3-5,7-8H,2,6H2,1H3

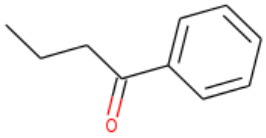
InChI Key: FFSAXUULYPJSKH-UHFFFAOYSA-N

Formula: C10H12O

SMILES: CCCC(=O)c1ccccc1

Molecular Weight: 148.20

CAS: 495-40-9



Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{liquid}$	-5461.30 ± 1.70	kJ/mol	NIST Webbook
$\Delta_f G°$	16.81	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-125.78	kJ/mol	Joback Method
$\Delta_f H°_{liquid}$	-188.80 ± 1.90	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	17.30	kJ/mol	Joback Method
$\Delta_{vap} H°$	46.88	kJ/mol	Joback Method
IE	9.10 ± 0.10	eV	NIST Webbook
IE	9.08	eV	NIST Webbook
IE	9.40 ± 0.20	eV	NIST Webbook
$logP_{oct/wat}$	2.67		Crippen Method
P_c	3142.03	kPa	Joback Method
T_{boil}	501.70	K	NIST Webbook
T_{boil}	395.00 ± 1.00	K	NIST Webbook
T_c	723.65	K	Joback Method
T_{fus}	278.81	K	Joback Method
V_c	0.49	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	276.61	J/mol×K	508.75	Joback Method
η	0.00	Pa×s	508.75	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H12O/c1-2-6-10(11)9-7-4-3-5-8-9/h3-5,7-8H,2,6H2,1H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

Δ_c**H°**$_{liquid}$: Standard liquid enthalpy of combustion (kJ/mol).
C$_{p,gas}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
Δ_f**G°**: Standard Gibbs free energy of formation (kJ/mol).
Δ_f**H°**$_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
Δ_f**H°**$_{liquid}$: Liquid phase enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{vap}**H°**: Enthalpy of vaporization at standard conditions (kJ/mol).
IE: Ionization energy (eV).
***log*P**$_{oct/wat}$: 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).