Benzoic acid, 3-nitro-

Other names: 3-Nitrobenzoic acid; Benzoic acid, m-nitro-; Metanitrobenzoic acid; m-Nitrobenzenecarboxylic acid; m-Nitrobenzoic acid.

InChI: InChI=1S/C7H5NO4/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4H,(H,9,10)

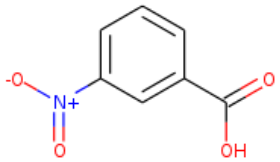
InChI Key: AFPHTEQTJZKQAQ-UHFFFAOYSA-N

Formula: C7H5NO4

SMILES: O=C(O)c1cccc([N+](=O)[O-])c1

Molecular Weight: 167.12

CAS: 121-92-6



Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{solid}$	-3055.00 ± 0.40	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-3053.24	kJ/mol	NIST Webbook
$\Delta_f G°$	-119.35	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-238.32	kJ/mol	Joback Method
$\Delta_f H°_{solid}$	-414.00 ± 0.40	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	24.59	kJ/mol	Joback Method
$\Delta_{sub} H°$	110.00 ± 0.40	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	74.13	kJ/mol	Joback Method
IE	10.30 ± 0.20	eV	NIST Webbook
$logP_{oct/wat}$	1.29		Crippen Method
P_c	5051.40	kPa	Joback Method
T_{boil}	689.11	K	Joback Method
T_c	923.22	K	Joback Method
T_{fus}	414.15 ± 1.50	K	NIST Webbook
T_{fus}	414.15 ± 1.50	K	NIST Webbook
T_{fus}	414.30 ± 0.30	K	NIST Webbook
V_c	0.43	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	268.39	J/mol×K	689.11	Joback Method
$C_{p,solid}$	179.90	J/mol×K	297.9	NIST Webbook
$C_{p,solid}$	173.20	J/mol×K	298.0	NIST Webbook
$C_{p,solid}$	201.70	J/mol×K	323.0	NIST Webbook
$\Delta_{fus}H$	21.40	kJ/mol	413.0	NIST Webbook
$\Delta_{fus}H$	19.33	kJ/mol	414.3	NIST Webbook
$\Delta_{fus}H$	19.33	kJ/mol	414.3	NIST Webbook
$\Delta_{fus}H$	19.33	kJ/mol	414.3	NIST Webbook
$\Delta_{sub}H$	107.20 ± 0.40	kJ/mol	354.0	NIST Webbook
$\Delta_{fus}S$	51.60	J/mol×K	413.0	NIST Webbook
$\Delta_{fus}S$	46.70	J/mol×K	414.3	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H5NO4/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4H,(H,9,10)
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

Δ_c**H°**$_{solid}$: Standard solid enthalpy of combustion (kJ/mol).
C$_{p,gas}$: Ideal gas heat capacity (J/mol×K).
C$_{p,solid}$: Solid phase heat capacity (J/mol×K).
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°**$_{solid}$: Solid phase enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{fus}**H**: Enthalpy of fusion at a given temperature (kJ/mol).
Δ_{sub}**H°**: Enthalpy of sublimation at standard conditions (kJ/mol).
Δ_{sub}**H**: Enthalpy of sublimation at a given temperature (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).
Δ_{fus}**S**: Entropy of fusion at a given temperature (J/mol×K).
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).