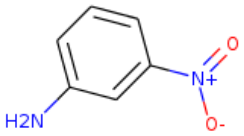
m-Nitroaniline

Other names: 1-Amino-3-nitrobenzene; 3-Aminonitrobenzene; 3-Nitroaniline; 3-Nitrobenzenamine; 3-Nitrobenzeneamine; 3-Nitrophenylamine; Amarthol Fast Orange R Base; Aniline, m-nitro-; Azobase MNA; Benzenamine, 3-nitro-; C.I. 37030; C.I. Azoic Diazo Component 7; Daito Orange Base R; Devol Orange R; Diazo Fast Orange R; Fast Orange Base R; Fast Orange M Base; Fast Orange MM Base; Fast Orange R Base; Fast Orange R Salt; Hiltonil Fast Orange R Base; MNA; NSC 9574; Naphtoelan Orange R Base; Nitranilin; Orange Base Irga I; m-Aminonitrobenzene; m-Nitraniline; m-Nitroaminobenzene; m-Nitrophenylamine.



InChI: InChI=1S/C6H6N2O2/c7-5-2-1-3-6(4-5)8(9)10/h1-4H,7H2

InChI Key: XJCVRTZCHMZPBD-UHFFFAOYSA-N

Formula: C6H6N2O2

SMILES: Nc1cccc([N+](=O)[O-])c1

Molecular Weight: 138.12

CAS: 99-09-2

Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{solid}$	-3184.32 ± 0.88	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-3180.00 ± 0.40	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-3190.30	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-3155.10	kJ/mol	NIST Webbook
EA	0.95 ± 0.10	eV	NIST Webbook
$\Delta_f G°$	204.42	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	62.50 ± 1.80	kJ/mol	NIST Webbook
$\Delta_f H°_{solid}$	-34.20 ± 1.20	kJ/mol	NIST Webbook
$\Delta_f H°_{solid}$	-38.00 ± 0.40	kJ/mol	NIST Webbook
$\Delta_f H°_{solid}$	-28.30	kJ/mol	NIST Webbook
$\Delta_f H°_{solid}$	-63.47	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	21.51	kJ/mol	Joback Method
$\Delta_{sub} H°$	97.00 ± 1.00	kJ/mol	NIST Webbook
$\Delta_{sub} H°$	96.50 ± 0.30	kJ/mol	NIST Webbook

Property	Value	Unit	Source
$\Delta_{vap}H°$	59.12	kJ/mol	Joback Method
IE	8.31 ± 0.02	eV	NIST Webbook
IE	8.80	eV	NIST Webbook
IE	8.60	eV	NIST Webbook
$log P_{oct/wat}$	1.18		Crippen Method
P_c	5037.07	kPa	Joback Method
T_{boil}	592.71	K	Joback Method
T_c	856.36	K	Joback Method
T_{fus}	387.65 ± 0.60	K	NIST Webbook
T_{fus}	384.95 ± 0.20	K	NIST Webbook
T_{fus}	387.00 ± 0.20	K	NIST Webbook
T_{fus}	382.65 ± 1.50	K	NIST Webbook
T_{fus}	385.00 ± 2.00	K	NIST Webbook
T_{fus}	385.00 ± 0.50	K	NIST Webbook
T_{fus}	385.00 ± 0.30	K	NIST Webbook
T_{fus}	387.80 ± 0.10	K	NIST Webbook
V_c	0.37	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	226.03	J/mol×K	592.71	Joback Method
$C_{p,solid}$	167.40	J/mol×K	297.9	NIST Webbook
$C_{p,solid}$	168.20	J/mol×K	298.0	NIST Webbook
$C_{p,solid}$	158.84	J/mol×K	298.15	NIST Webbook
$C_{p,solid}$	186.60	J/mol×K	323.0	NIST Webbook
$\Delta_{fus}H$	23.60	kJ/mol	384.95	NIST Webbook
$\Delta_{fus}H$	23.68	kJ/mol	385.0	NIST Webbook

Property	Value	Unit	Temperature (K)	Source
$\Delta_{fus}H$	23.69	kJ/mol	387.0	NIST Webbook
$\Delta_{fus}H$	23.68	kJ/mol	387.0	NIST Webbook
$\Delta_{fus}H$	23.68	kJ/mol	387.2	NIST Webbook
$\Delta_{sub}H$	97.50 ± 4.20	kJ/mol	288.0	NIST Webbook
$\Delta_{sub}H$	97.60	kJ/mol	315.5	NIST Webbook
$\Delta_{sub}H$	88.70 ± 2.50	kJ/mol	336.5	NIST Webbook
$\Delta_{sub}H$	88.30 ± 1.70	kJ/mol	336.5	NIST Webbook
$\Delta_{sub}H$	89.00 ± 2.00	kJ/mol	342.0	NIST Webbook
$\Delta_{sub}H$	93.60 ± 0.70	kJ/mol	352.0	NIST Webbook
$\Delta_{sub}H$	94.60 ± 0.30	kJ/mol	352.0	NIST Webbook
$\Delta_{vap}H$	64.90	kJ/mol	510.5	NIST Webbook
$\Delta_{fus}S$	61.30	J/mol×K	384.95	NIST Webbook
$\Delta_{fus}S$	61.50	J/mol×K	385.0	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H6N2O2/c7-5-2-1-3-6(4-5)8(9)10/h1-4H,7H2
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\Delta_c\mathbf{H°_{solid}}$: Standard solid enthalpy of combustion (kJ/mol).
$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{C_{p,solid}}$: Solid phase heat capacity (J/mol×K).
EA: Electron affinity (eV).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_f\mathbf{H°_{solid}}$: Solid phase enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H}$: Enthalpy of fusion at a given temperature (kJ/mol).
$\Delta_{sub}\mathbf{H°}$: Enthalpy of sublimation at standard conditions (kJ/mol).
$\Delta_{sub}\mathbf{H}$: Enthalpy of sublimation at a given temperature (kJ/mol).

Δ_{vap}**H°**: Enthalpy of vaporization at standard conditions (kJ/mol).
Δ_{vap}**H**: Enthalpy of vaporization at a given temperature (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).