Benzoic acid, 4-nitro-, methyl ester

Other names: 4-Nitrobenzoic acid methyl ester; Benzoic acid, p-nitro-, methyl ester; Methyl 4-nitrobenzoate; Methyl ester of 4-Nitrobenzoic acid; Methyl p-nitrobenzoate; Methyl para-nitrobenzoate; p-Nitrobenzoic acid methyl ester.

InChI: InChI=1S/C8H7NO4/c1-13-8(10)6-2-4-7(5-3-6)9(11)12/h2-5H,1H3

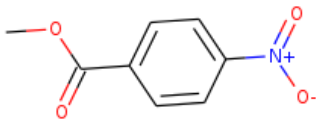
InChI Key: YOJAHJGBFDPSDI-UHFFFAOYSA-N

Formula: C8H7NO4

SMILES: COC(=O)c1ccc([N+](=O)[O-])cc1

Molecular Weight: 181.15

CAS: 619-50-1



Physical Properties

Property	Value	Unit	Source
PAff	813.20	kJ/mol	NIST Webbook
BasG	782.30	kJ/mol	NIST Webbook
EA	1.46 ± 0.09	eV	NIST Webbook
EA	1.47 ± 0.09	eV	NIST Webbook
$\Delta_f G°$	-79.11	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-287.00 ± 11.00	kJ/mol	NIST Webbook
$\Delta_f H°_{liquid}$	-387.20 ± 1.30	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	24.28	kJ/mol	Joback Method
$\Delta_{vap} H°$	100.00 ± 10.00	kJ/mol	NIST Webbook
IE	9.70	eV	NIST Webbook
$logP_{oct/wat}$	1.38		Crippen Method
P_c	3848.31	kPa	Joback Method
T_{boil}	642.23	K	Joback Method
T_c	889.97	K	Joback Method
T_{fus}	434.63	K	Joback Method
V_c	0.48	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	298.26	J/mol×K	642.23	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H7NO4/c1-13-8(10)6-2-4-7(5-3-6)9(11)12/h2-5H,1H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

PAff: Proton affinity (kJ/mol).
BasG: Gas basicity (kJ/mol).
$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
EA: Electron affinity (eV).
$\Delta_f G°$: 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).
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).