p-Nitroaniline

Other names:

1-Amino-4-nitrobenzene
4-Aminonitrobenzene
4-Nitraniline
4-Nitroaniline
4-Nitrobenzenamine
Aniline, 4-nitro-
Aniline, p-nitro-
Azoamine Red 2H
Azoamine Red Zh
Azofix Red GG Salt
Azoic Diazo Component 37
Benzenamine, 4-nitro-
C.I. 37035
C.I. Azoic Diazo Component 37
C.I. Developer 17
Developer P
Devol Red GG
Diazo Fast Red GG
Fast Red 2G Base
Fast Red 2G Salt
Fast Red Base 2J
Fast Red Base GG
Fast Red GG Base
Fast Red GG Salt
Fast Red MP Base
Fast Red P Base
Fast Red P Salt
Fast Red Salt 2J
Fast Red Salt GG
NCI-C60786
NSC 9797
Naphtoelan Red GG Base
Nitrazol CF extra
PNA
Paranitroaniline
Rcra waste number P077
Red 2G Base
Shinnippon Fast Red GG Base
aniline, p-nitro
p-Aminonitrobenzene

p-Nitraniline
p-Nitroanilina
p-Nitrophenylamine

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

InchiKey: TYMLOMAKGOJONV-UHFFFAOYSA-N

Formula: C6H6N2O2

SMILES: Nc1ccc([N+](=O)[O-])cc1

Mol. weight [g/mol]: 138.12

CAS: 100-01-6

Physical Properties

Property code	Value	Unit	Source
affp	866.00	kJ/mol	NIST Webbook
basg	834.20	kJ/mol	NIST Webbook
chs	-3180.00 ± 3.20	kJ/mol	NIST Webbook
chs	-3176.00 ± 0.80	kJ/mol	NIST Webbook
chs	-3177.10	kJ/mol	NIST Webbook
chs	-3172.98 ± 0.90	kJ/mol	NIST Webbook
ea	0.75 ± 0.10	eV	NIST Webbook
ea	0.92 ± 0.09	eV	NIST Webbook
gf	204.42	kJ/mol	Joback Method
hf	55.20 ± 1.80	kJ/mol	NIST Webbook
hfs	-45.60 ± 1.20	kJ/mol	NIST Webbook
hfs	-43.10 ± 0.80	kJ/mol	NIST Webbook
hfs	-38.50 ± 3.20	kJ/mol	NIST Webbook
hfs	-41.50	kJ/mol	NIST Webbook
hfus	21.51	kJ/mol	Joback Method
hvap	59.12	kJ/mol	Joback Method
ie	8.60	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
ie	8.43	eV	NIST Webbook
ie	8.34 ± 0.01	eV	NIST Webbook
ie	8.60 ± 0.10	eV	NIST Webbook
log10ws	-2.37		Estimated Solubility Method
log10ws	-2.37		Aqueous Solubility Prediction Method
logp	1.177		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=3)		KDB

nfpas	%!d(float64=3)		KDB
pc	5037.07	kPa	Joback Method
rinpol	273.60		NIST Webbook
rinpol	273.75		NIST Webbook
rinpol	273.75		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1560.00		NIST Webbook
tb	592.71	K	Joback Method
tc	856.36	K	Joback Method
tf	420.15	K	KDB
tf	421.05	K	Aqueous Solubility Prediction Method
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.34	J/mol×K	856.36	Joback Method
cpg	235.82	J/mol×K	636.65	Joback Method
cpg	244.79	J/mol×K	680.59	Joback Method
cpg	252.98	J/mol×K	724.54	Joback Method
cpg	260.43	J/mol×K	768.48	Joback Method
cpg	267.21	J/mol×K	812.42	Joback Method
cpg	226.03	J/mol×K	592.71	Joback Method
cps	154.20	J/mol×K	298.15	NIST Webbook
cps	184.90	J/mol×K	323.00	NIST Webbook
cps	169.00	J/mol×K	298.00	NIST Webbook
cps	165.70	J/mol×K	297.90	NIST Webbook
hfust	21.09	kJ/mol	420.70	NIST Webbook
hfust	21.15	kJ/mol	420.65	NIST Webbook
hfust	21.09	kJ/mol	420.70	NIST Webbook
hfust	21.09	kJ/mol	420.20	NIST Webbook
hsubt	103.30 ± 1.70	kJ/mol	362.00	NIST Webbook
hsubt	97.50 ± 1.70	kJ/mol	356.00	NIST Webbook
hsubt	98.70 ± 2.50	kJ/mol	361.00	NIST Webbook
hsubt	109.30	kJ/mol	333.00	NIST Webbook
hsubt	109.20 ± 4.20	kJ/mol	303.00	NIST Webbook
hsubt	99.00 ± 3.00	kJ/mol	361.00	NIST Webbook
hvapt	77.90	kJ/mol	505.50	NIST Webbook
hvapt	70.00	kJ/mol	512.00	NIST Webbook

psub	2.05e-03	kPa	363.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range	
psub	3.20e-05	kPa	323.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range	
psub	2.98e-04	kPa	343.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range	
psub	0.10	kPa	413.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range	
psub	0.05	kPa	403.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range	
psub	0.01	kPa	383.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range	
sfust	50.10	J/mol×K	420.70	NIST Webbook	
sfust	50.30	J/mol×K	420.65	NIST Webbook	

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	533.20	K	13.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.70988e+01
Coeff. B	-6.95603e+03
Coeff. C	-5.17590e+01
Temperature range (K), min.	420.65
Temperature range (K), max.	641.89

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-7.53103e+01
Coeff. B	-4.12308e+03
Coeff. C	1.40535e+01
Coeff. D	-9.31048e-06
Temperature range (K), min.	420.65
Temperature range (K), max.	658.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range:	https://www.doi.org/10.1016/j.tca.2010.11.034
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Solubility of p-Nitroaniline in Supercritical Carbon Dioxide with and without Mixed Cosolvents:	https://www.doi.org/10.1021/je300987d

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1291
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1291
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Solid-Liquid Phase Diagram of the Ternary System of p-Nitroaniline + o-Nitroaniline + Ethanol:	https://www.doi.org/10.1021/je1005104
McGowanMethod:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100016&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume