2-Nitroaniline

Other names:

1-Nitro-2-aminobenzene
1-amino-2-nitrobenzene
2-Aminonitrobenzene
2-Nitro-benzeneamine
2-Nitrobenzenamine
Aniline, o-nitro-
Azoene Fast Orange GR Base
Azoene Fast Orange GR Salt
Azofix Orange GR Salt
Azogene Fast Orange GR
Azoic Diazo Component 6
Benzenamine, 2-nitro-
Brentamine Fast Orange GR Base
Brentamine Fast Orange GR Salt
C.I. 37025
C.I. Azoic Diazo Component 6
Devol Orange B
Devol Orange Salt B
Diazo Fast Orange GR
Fast Orange Base GR
Fast Orange Base JR
Fast Orange GR Base
Fast Orange GR Salt
Fast Orange O Base
Fast Orange O Salt
Fast Orange Salt GR
Fast Orange Salt JR
Hiltonil Fast Orange GR Base
Hiltosal Fast Orange GR Salt
Hindasol Orange GR Salt
NSC 9796
Natasol Fast Orange GR Salt
ONA
Orange Base Ciba II
Orange Base Irga II
Orange GRS Salt
Orange Salt Ciba II
Orange Salt Irga II
Orthonitroaniline
o-Aminonitrobenzene

	o-Nitranilin
	o-Nitraniline
	o-nitroaniline
Inchi:	InChI=1S/C6H6N2O2/c7-5-3-1-2-4-6(5)8(9)10/h1-4H,7H2
InchiKey:	DPJCXCZTLWNFOH-UHFFFAOYSA-N
Formula:	C6H6N2O2
SMILES:	Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	138.13
CAS:	88-74-4

Physical Properties

Property code	Value	Unit	Source
chs	-3192.30	kJ/mol	NIST Webbook
chs	-3192.00 ± 0.40	kJ/mol	NIST Webbook
hf	71.80	kJ/mol	Cheméo Relay (1.0)
hfs	-26.30	kJ/mol	NIST Webbook
hfs	-26.00 ± 0.40	kJ/mol	NIST Webbook
hfus	21.51	kJ/mol	Joback Method
hsub	89.00 ± 0.70	kJ/mol	NIST Webbook
hvap	64.48	kJ/mol	Cheméo Relay (1.0)
ie	8.66	eV	NIST Webbook
ie	8.43	eV	NIST Webbook
ie	8.27 ± 0.01	eV	NIST Webbook
log10ws	-1.96		Estimated Solubility Method
log10ws	-1.96		Aqueous Solubility Prediction Method
logp	1.177		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
rinpol	1402.00		NIST Webbook
rinpol	241.10		NIST Webbook
rinpol	241.10		NIST Webbook
tb	557.20	K	NIST Webbook
tf	342.90 ± 0.10	K	NIST Webbook
tf	342.45 ± 0.30	K	NIST Webbook
tf	344.60 ± 0.15	K	NIST Webbook
tf	342.00 ± 1.50	K	NIST Webbook
tf	343.75 ± 0.30	K	NIST Webbook
tf	344.30 ± 0.20	K	NIST Webbook
tf	344.15 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.03	J/mol×K	592.71	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	273.34	J/mol×K	856.36	Joback Method
cps	164.40	J/mol×K	298.00	NIST Webbook
cps	168.20	J/mol×K	297.90	NIST Webbook
hfust	16.11	kJ/mol	342.50	NIST Webbook
hfust	16.11	kJ/mol	342.50	NIST Webbook
hfust	16.11	kJ/mol	344.40	NIST Webbook
hsubt	87.20 ± 0.70	kJ/mol	327.50	NIST Webbook
hsubt	79.90 ± 1.70	kJ/mol	314.50	NIST Webbook
hsubt	82.00 ± 2.00	kJ/mol	313.00	NIST Webbook
hsubt	82.00 ± 2.00	kJ/mol	313.00	NIST Webbook
hsubt	90.00 ± 4.20	kJ/mol	223.00	NIST Webbook
hvapt	64.80	kJ/mol	467.50	NIST Webbook
hvapt	59.30	kJ/mol	488.00	NIST Webbook
psub	1.89e-03	kPa	323.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	3.23e-03	kPa	328.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range

psub	8.82e-03	kPa	338.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	1.09e-03	kPa	318.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	6.21e-04	kPa	313.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	3.64e-04	kPa	308.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
sfust	47.00	J/mol×K	342.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.71477e+01
Coeff. B	-6.49919e+03
Coeff. C	-3.84840e+01
Temperature range (K), min.	423.96
Temperature range (K), max.	587.58

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.36243e+02
Coeff. B	-1.36758e+04
Coeff. C	-1.74694e+01
Coeff. D	1.08034e-05
Temperature range (K), min.	344.65
Temperature range (K), max.	600.15

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1289
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Cheméo Relay (1.0, beta):	
New method for determination of vaporization and sublimation enthalpy of aromatic compounds at 298.15 K using solution calorimetry technique and group-additivity scheme:	https://www.doi.org/10.1016/j.tca.2015.09.022
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0):	
Solid-Liquid Phase Diagram of the Ternary System of p-Nitroaniline + o-Nitroaniline + Ethanol:	https://www.doi.org/10.1021/je1005104
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1289
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88744&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
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
hsub:	Enthalpy of sublimation at standard conditions
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
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point