

o-Nitroaniline

Other names:	1-Amino-2-Nitrobenzene
	1-Nitro-2-aminobenzene
	2-Aminonitrobenzene
	2-Nitro-benzeneamine
	2-Nitroaniline
	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
Inchi: InChI=1S/C6H6N2O2/c7-5-3-1-2-4-6(5)8(9)10/h1-4H,7H2
InchiKey: DPJXCXCZTLWNFOH-UHFFFAOYSA-N
Formula: C6H6N2O2
SMILES: Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 138.12
CAS: 88-74-4

Physical Properties

Property code	Value	Unit	Source
chs	-3192.00 ± 0.40	kJ/mol	NIST Webbook
chs	-3192.30	kJ/mol	NIST Webbook
gf	204.42	kJ/mol	Joback Method
hf	80.92	kJ/mol	Joback Method
hfs	-26.00 ± 0.40	kJ/mol	NIST Webbook
hfs	-26.30	kJ/mol	NIST Webbook
hfus	21.51	kJ/mol	Joback Method
hsub	89.00 ± 0.70	kJ/mol	NIST Webbook
hvap	59.12	kJ/mol	Joback Method
ie	8.27 ± 0.01	eV	NIST Webbook
ie	8.66	eV	NIST Webbook
ie	8.43	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
pc	5037.07	kPa	Joback Method
rinpol	1402.00		NIST Webbook
rinpol	241.10		NIST Webbook
rinpol	241.10		NIST Webbook
tb	557.20	K	NIST Webbook
tc	856.36	K	Joback Method
tf	344.60 ± 0.15	K	NIST Webbook
tf	344.15 ± 0.50	K	NIST Webbook
tf	344.30 ± 0.20	K	NIST Webbook
tf	343.75 ± 0.30	K	NIST Webbook
tf	342.00 ± 1.50	K	NIST Webbook

tf	342.45 ± 0.30	K	NIST Webbook
tf	342.90 ± 0.10	K	NIST Webbook
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	267.21	J/mol×K	812.42	Joback Method
cpg	260.43	J/mol×K	768.48	Joback Method
cpg	252.98	J/mol×K	724.54	Joback Method
cpg	244.79	J/mol×K	680.59	Joback Method
cpg	235.82	J/mol×K	636.65	Joback Method
cpg	226.03	J/mol×K	592.71	Joback Method
cps	168.20	J/mol×K	297.90	NIST Webbook
cps	164.40	J/mol×K	298.00	NIST Webbook
hfust	16.11	kJ/mol	344.40	NIST Webbook
hfust	16.11	kJ/mol	342.50	NIST Webbook
hfust	16.11	kJ/mol	342.50	NIST Webbook
hsubt	87.20 ± 0.70	kJ/mol	327.50	NIST Webbook
hsubt	90.00 ± 4.20	kJ/mol	223.00	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	79.90 ± 1.70	kJ/mol	314.50	NIST Webbook
hvapt	64.80	kJ/mol	467.50	NIST Webbook
hvapt	59.30	kJ/mol	488.00	NIST Webbook
psub	3.64e-04	kPa	308.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
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	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	8.82e-03	kPa	338.15	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
sfust	47.00	J/mol×K	342.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88744&Units=SI
KDB Vapor Pressure Data:	https://www.thermopedia.com/research/kdb/hcprop/showprop.php?cmpid=1289
KDB:	https://www.thermopedia.com/research/kdb/hcprop/showprop.php?cmpid=1289
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation	https://www.doi.org/10.1016/j.tca.2010.11.034
Solid-Liquid Phase Diagram of the Triacetone triperoxide + Ethanol System	https://www.doi.org/10.1021/je1005104
Temperature range: 344.65 K - 600.15 K	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
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
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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/35-381-0/o-Nitroaniline.pdf>

Generated by Cheméo on 2025-12-23 01:47:22.359258523 +0000 UTC m=+6202639.889299177.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.