Benzene, 1-chloro-2-nitro-

Other names:	1-Chloro-2-Nitrobenzene
	1-Nitro-2-chlorobenzene
	2-Chloro-1-nitrobenzene
	2-Chloronitrobenzene
	2-Nitro-1-chlorobenzene
	2-Nitrochlorobenzene
	Chloro-o-nitrobenzene
	NSC 36934
	Nitrochlorobenzene, o-
	Nitrochlorobenzene, ortho
	O-NITROPHENYL CHLORIDE
	ONCB
	o-Chloronitrobenzene
	o-Nitrochlorobenzene
Inchi:	InChI=1S/C6H4ClNO2/c7-5-3-1-2-4-6(5)8(9)10/h1-4H
InchiKey:	BFCFYVKQTRLZHA-UHFFFAOYSA-N
Formula:	C6H4ClNO2
SMILES:	O=[N+]([O-])c1ccccc1Cl
Mol. weight [g/mol]:	157.55
CAS:	88-73-3

Physical Properties

Property code	Value	Unit	Source
chs	-2923.30 ± 2.50	kJ/mol	NIST Webbook
ea	1.16 ± 0.10	eV	NIST Webbook
ea	1.11 ± 0.05	eV	NIST Webbook
ea	1.34 ± 0.05	eV	NIST Webbook
gf	126.04	kJ/mol	Joback Method
hf	31.39	kJ/mol	Joback Method
hfs	-32.90	kJ/mol	NIST Webbook
hfus	18.11	kJ/mol	Heat Capacities of Chloroanilines and Chloronitrobenzenes
hsub	80.80 ± 0.30	kJ/mol	NIST Webbook
hsub	80.90 ± 1.50	kJ/mol	NIST Webbook
hvap	60.40 ± 0.30	kJ/mol	NIST Webbook
log10ws	-2.55		Aqueous Solubility Prediction Method

log10ws	-2.55		Estimated Solubility Method
logp	2.248		Crippen Method
mcvol	101.300	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=3)		KDB
nfpas	%!d(float64=1)		KDB
pc	4426.72	kPa	Joback Method
rinpol	1241.00		NIST Webbook
rinpol	213.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1199.00		NIST Webbook
ripol	1946.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1946.00		NIST Webbook
tb	519.15 ± 0.60	K	NIST Webbook
tb	519.20	K	NIST Webbook
tc	817.38	K	Joback Method
tf	305.28 ± 0.07	K	NIST Webbook
tf	305.70 ± 1.50	K	NIST Webbook
tf	305.15 ± 0.15	K	NIST Webbook
tf	306.00 ± 1.50	K	NIST Webbook
tf	305.28 ± 0.05	K	NIST Webbook
tf	306.03	K	Aqueous Solubility Prediction Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.06	J/mol×K	557.61	Joback Method
cpg	209.08	J/mol×K	600.91	Joback Method
cpg	217.33	J/mol×K	644.20	Joback Method
cpg	224.86	J/mol×K	687.50	Joback Method
cpg	231.72	J/mol×K	730.79	Joback Method
cpg	237.94	J/mol×K	774.09	Joback Method
cpg	243.57	J/mol×K	817.38	Joback Method
hfust	18.11	kJ/mol	305.80	NIST Webbook
hfust	18.21	kJ/mol	305.80	NIST Webbook
hfust	19.08	kJ/mol	308.20	NIST Webbook
hvapt	52.10	kJ/mol	468.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.20	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50943e+01
Coeff. B	-4.62238e+03
Coeff. C	-7.77630e+01
Temperature range (K), min.	389.94
Temperature range (K), max.	550.26

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.11244e+02
Coeff. B	-1.20614e+04
Coeff. C	-1.35369e+01
Coeff. D	4.71347e-06
Temperature range (K), min.	306.15
Temperature range (K), max.	757.00

Sources

Heat Capacities of Chloroanilines and Chloronitrobenzenes:	https://www.doi.org/10.1021/je700080k
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=1795
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1795
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88733&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume