Benzene, 1-chloro-3-nitro-

Other names:	1-Chloro-3-nitrobenzene
	3-Chloro-1-nitrobenzene
	3-Chloronitrobenzene
	Chloro-m-nitrobenzene
	M-NITROPHENYL CHLORIDE
	Metachloronitrobenzene
	NSC 5502
	Nitrochlorobenzene, meta-
	m-Chloronitrobenzene
	m-Nitrochlorobenzene
Inchi:	InChI=1S/C6H4ClNO2/c7-5-2-1-3-6(4-5)8(9)10/h1-4H
InchiKey:	KMAQZIILEGKYQZ-UHFFFAOYSA-N
Formula:	C6H4ClNO2
SMILES:	O=[N+]([O-])c1cccc(Cl)c1
Mol. weight [g/mol]:	157.55
CAS:	121-73-3

Physical Properties

Property code	Value	Unit	Source
chs	-2899.00 ± 3.00	kJ/mol	NIST Webbook
ea	1.28 ± 0.10	eV	NIST Webbook
ea	1.26 ± 0.05	eV	NIST Webbook
ea	1.38 ± 0.05	eV	NIST Webbook
ea	1.26 ± 0.09	eV	NIST Webbook
gf	126.04	kJ/mol	Joback Method
hf	31.39	kJ/mol	Joback Method
hfs	-58.99	kJ/mol	NIST Webbook
hfus	19.52	kJ/mol	Heat Capacities of Chloroanilines and Chloronitrobenzenes
hsub	82.50 ± 1.50	kJ/mol	NIST Webbook
hsub	81.30 ± 0.30	kJ/mol	NIST Webbook
hvap	60.20 ± 0.20	kJ/mol	NIST Webbook
ie	9.90 ± 0.10	eV	NIST Webbook
log10ws	-2.77		Estimated Solubility Method
log10ws	-2.77		Aqueous Solubility Prediction Method

logp	2.248		Crippen Method
mcvol	101.300	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
rinpol	1185.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	210.00		NIST Webbook
ripol	1847.00		NIST Webbook
ripol	1862.00		NIST Webbook
ripol	1847.00		NIST Webbook
tb	508.65 ± 0.60	K	NIST Webbook
tb	508.70	K	NIST Webbook
tc	817.38	K	Joback Method
tf	316.95 ± 0.60	K	NIST Webbook
tf	317.90	K	Aqueous Solubility Prediction Method
tf	297.15	K	KDB
tf	317.00 ± 1.50	K	NIST Webbook
tf	316.30 ± 0.60	K	NIST Webbook
tf	317.00 ± 2.00	K	NIST Webbook
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.57	J/mol×K	817.38	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	200.06	J/mol×K	557.61	Joback Method
hfust	19.52	kJ/mol	316.90	NIST Webbook
hfust	18.65	kJ/mol	318.00	NIST Webbook
hfust	19.37	kJ/mol	317.60	NIST Webbook
hsubt	75.00 ± 2.00	kJ/mol	281.00	NIST Webbook
hsubt	74.70 ± 1.70	kJ/mol	280.50	NIST Webbook
hvapt	51.50	kJ/mol	460.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50719e+01
Coeff. B	-4.50563e+03
Coeff. C	-7.77390e+01
Temperature range (K), min.	382.50
Temperature range (K), max.	539.36

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.11915e+02
Coeff. B	-1.18294e+04
Coeff. C	-1.37033e+01
Coeff. D	5.23943e-06
Temperature range (K), min.	317.65
Temperature range (K), max.	742.00

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1796

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C121733&Units=SI

Heat Capacities of Chloroanilines and Chloronitrobenzenes: https://www.doi.org/10.1021/je700080k

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1796

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume