Benzene, 1-chloro-4-nitro-

Other names:	1-Chloor-4-nitrobenzeen
	1-Chlor-4-nitrobenzol
	1-Chloro-4-nitrobenzene
	1-Cloro-4-nitrobenzene
	1-Nitro-4-chlorobenzene
	4-Chloro-1-nitrobenzene
	4-Chloronitrobenzene
	4-Nitro-1-chlorobenzene
	4-Nitrochlorobenzene
	NSC 9792
	Nitrochlorobenzene, p-
	Nitrochlorobenzene, para
	PNCB
	p-Chloronitrobenzene
	p-Nitrochloorbenzeen
	p-Nitrochlorobenzene
	p-Nitrochlorobenzol
	p-Nitroclorobenzene
	p-Nitrophenyl chloride
Inchi:	InChI=1S/C6H4ClNO2/c7-5-1-3-6(4-2-5)8(9)10/h1-4H
InchiKey:	CZGCEKJOLUNIFY-UHFFFAOYSA-N
Formula:	C6H4ClNO2
SMILES:	O=[N+]([O-])c1ccc(Cl)cc1
Mol. weight [g/mol]:	157.55
CAS:	100-00-5

Physical Properties

Property code	Value	Unit	Source
chs	-2907.50 ± 3.20	kJ/mol	NIST Webbook
ea	1.27 ± 0.05	eV	NIST Webbook
ea	1.23 ± 0.05	eV	NIST Webbook
ea	1.26 ± 0.10	eV	NIST Webbook
ea	1.23 ± 0.09	eV	NIST Webbook
gf	126.04	kJ/mol	Joback Method
hf	31.39	kJ/mol	Joback Method
hfs	-48.74	kJ/mol	NIST Webbook

hfus	15.03	kJ/mol	Heat Capacities of Chloroanilines and Chloronitrobenzenes
hsub	74.70 ± 0.10	kJ/mol	NIST Webbook
hvap	52.86	kJ/mol	Joback Method
ie	9.99	eV	NIST Webbook
ie	10.00 ± 0.10	eV	NIST Webbook
log10ws	-2.92		Estimated Solubility Method
log10ws	-2.92		Aqueous Solubility Prediction Method
logp	2.248		Crippen Method
mcvol	101.300	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=3)		KDB
pc	4426.72	kPa	Joback Method
rinpol	1187.00		NIST Webbook
rinpol	212.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1187.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1189.00		NIST Webbook
ripol	1887.00		NIST Webbook
ripol	1887.00		NIST Webbook
ripol	1887.00		NIST Webbook
ripol	1902.00		NIST Webbook
tb	515.20	K	NIST Webbook
tb	512.25 ± 0.60	K	NIST Webbook
tb	512.25 ± 0.50	K	NIST Webbook
tc	817.38	K	Joback Method
tf	356.87	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	237.94	J/mol×K	774.09	Joback Method
cpg	231.72	J/mol×K	730.79	Joback Method
cpg	224.86	J/mol×K	687.50	Joback Method
cpg	217.33	J/mol×K	644.20	Joback Method

cpg	209.08	J/mol×K	600.91	Joback Method
cpg	243.57	J/mol×K	817.38	Joback Method
cps	250.20	J/mol×K	298.00	NIST Webbook
hfust	15.03	kJ/mol	355.10	NIST Webbook
hfust	16.17	kJ/mol	356.10	NIST Webbook
hfust	11.85	kJ/mol	354.60	NIST Webbook
hfust	14.10	kJ/mol	357.00	NIST Webbook
hfust	18.03	kJ/mol	358.00	NIST Webbook
hfust	11.85	kJ/mol	354.60	NIST Webbook
hsubt	83.20	kJ/mol	293.00	NIST Webbook
hvapt	36.90	kJ/mol	518.00	NIST Webbook
hvapt	51.30	kJ/mol	450.00	NIST Webbook
sfust	33.40	J/mol×K	354.60	NIST Webbook
sfust	69.90	J/mol×K	358.00	NIST Webbook
svapt	71.20	J/mol×K	518.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	386.20	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50426e+01
Coeff. B	-4.49846e+03
Coeff. C	-8.36130e+01
Temperature range (K), min.	388.49
Temperature range (K), max.	545.89

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.86377e+02
Coeff. B	-1.58816e+04

Coeff. C	-2.46220e+01
Coeff. D	1.08367e-05
Temperature range (K), min.	356.65
Temperature range (K), max.	751.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100005&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1797
Heat Capacities of Chloroanilines and Chloronitrobenzenes:	https://www.doi.org/10.1021/je700080k
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1797
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
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
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
sfust:	Entropy of fusion at a given temperature
svapt:	Entropy of vaporization 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