Benzene, 1-chloro-4-isocyanato-

Other names:	1-Chloro-4-isocyanatobenzene
	4-Chloro-iso-cyanatobenzene
	4-Chlorophenyl isocyanate
	Isocyanic acid, p-chlorophenyl ester
	NSC 76589
	PCPI
	p-Chlorfenylisokyanat
	p-Chlorophenyl isocyanate
	para-Chlorophenyl isocyanate
Inchi:	InChI=1S/C7H4ClNO/c8-6-1-3-7(4-2-6)9-5-10/h1-4H
InchiKey:	ADAKRBAJFHTIEW-UHFFFAOYSA-N
Formula:	C7H4ClNO
SMILES:	O=C=Nc1ccc(Cl)cc1
Mol. weight [g/mol]:	153.57
CAS:	104-12-1

Physical Properties

Property code	Value	Unit	Source
chl	-3320.50 ± 5.10	kJ/mol	NIST Webbook
chs	-3259.00 ± 4.20	kJ/mol	NIST Webbook
hf	16.10	kJ/mol	Joback Method
hfs	-83.70 ± 4.20	kJ/mol	NIST Webbook
hvap	49.80 ± 0.20	kJ/mol	NIST Webbook
ie	8.80 ± 0.10	eV	NIST Webbook
log10ws	-6.64		Crippen Method
logp	2.307		Crippen Method
mcvol	105.220	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
rinpol	1100.00		NIST Webbook
tb	495.32	K	Joback Method
tc	727.09	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	210.90	J/mol×K	282.00	NIST Webbook
hvapt	48.90	kJ/mol	403.00	NIST Webbook
hvapt	44.30	kJ/mol	378.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	3.21752e+01
Coeff. B	-2.42416e+04
Coeff. C	4.03048e+02
Temperature range (K), min.	323.00
Temperature range (K), max.	499.35

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C104121&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chl: Standard liquid enthalpy of combustion

chs: Standard solid enthalpy of combustion

cps: Solid phase heat capacity

hf: Enthalpy of formation at standard conditions

hfs: Solid phase enthalpy of formation at standard conditions

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature