

Benzene, 1-chloro-3-isocyanato-

Other names:	1-Chloro-3-isocyanatobenzene 3-Chloroisocyanatobenzene 3-Chlorophenyl isocyanate Isocyanic acid, m-chlorophenyl ester m-Chlorfenylisokyanat m-Chlorophenyl isocyanate
Inchi:	InChI=1S/C7H4ClNO/c8-6-2-1-3-7(4-6)9-5-10/h1-4H
InchiKey:	HHIRBXHEYVDUAM-UHFFFAOYSA-N
Formula:	C7H4ClNO
SMILES:	O=C=Nc1cccc(Cl)c1
Mol. weight [g/mol]:	153.57
CAS:	2909-38-8

Physical Properties

Property code	Value	Unit	Source
chl	-3277.00 ± 64.00	kJ/mol	NIST Webbook
chs	-3264.00 ± 4.20	kJ/mol	NIST Webbook
hf	16.10	kJ/mol	Joback Method
hfs	-82.80 ± 4.20	kJ/mol	NIST Webbook
hvap	54.00 ± 0.20	kJ/mol	NIST Webbook
ie	9.00 ± 0.10	eV	NIST Webbook
log10ws	-6.64		Crippen Method
logp	2.307		Crippen Method
mvol	105.220	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
tb	495.32	K	Joback Method
tc	727.09	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	187.00	J/mol×K	294.20	NIST Webbook
hvapt	53.10	kJ/mol	388.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.35996e+01
Coeff. B	-3.39408e+03
Coeff. C	-9.59960e+01
Temperature range (K), min.	344.00
Temperature range (K), max.	505.50

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
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2909388&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpl:	Liquid 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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure

pvap: Vapor pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature

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