Cyanogen chloride

Other names:	CHLORINE CYANIDE
	CHLOROCYAN
	CHLOROCYANIDE
	CK
	CNCl
	Chlorcyan
	Chlorine cyanide (ClCN)
	Chlorocyanide (ClCN)
	Chlorocyanogen
	Chlorure de cyanogene
	ClCN
	Cyanochloride
	Cyanochloride (CNCll)
	Cyanogen chloride ((CN)Cl)
	Cyanogen chloride (ClCN)
	Rcra waste number P033
Inchi:	InChI=1S/CClN/c2-1-3
InchiKey:	QPJDMGCKMHUXFD-UHFFFAOYSA-N
Formula:	CClN
SMILES:	N#CCl
Mol. weight [g/mol]:	61.47
CAS:	506-77-4

Physical Properties

Property code	Value	Unit	Source
affp	722.10	kJ/mol	NIST Webbook
basg	691.50	kJ/mol	NIST Webbook
gf	78.79	kJ/mol	Joback Method
hf	85.17	kJ/mol	Joback Method
hfs	137.80 ± 4.20	kJ/mol	NIST Webbook
hfus	4.05	kJ/mol	Joback Method
hvap	32.68	kJ/mol	Joback Method
ie	12.34 ± 0.01	eV	NIST Webbook
ie	12.36 ± 0.02	eV	NIST Webbook
ie	12.37	eV	NIST Webbook
ie	12.34	eV	NIST Webbook
ie	12.37 ± 0.02	eV	NIST Webbook

log10ws	-0.76		Crippen Method
logp	0.706		Crippen Method
mcvol	38.570	ml/mol	McGowan Method
pc	5281.57	kPa	Joback Method
tb	286.15	K	KDB
tc	566.73	K	Joback Method
tf	266.65	K	KDB
vc	0.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	44.03	J/mol×K	361.79	Joback Method
cpg	44.94	J/mol×K	395.95	Joback Method
cpg	45.82	J/mol×K	430.10	Joback Method
cpg	46.66	J/mol×K	464.26	Joback Method
cpg	47.46	J/mol×K	498.41	Joback Method
cpg	48.23	J/mol×K	532.57	Joback Method
cpg	48.96	J/mol×K	566.73	Joback Method
hsubt	35.70	kJ/mol	227.50	NIST Webbook
hvapt	32.20	kJ/mol	241.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42163e+01
Coeff. B	-2.10447e+03
Coeff. C	-6.67380e+01
Temperature range (K), min.	217.83
Temperature range (K), max.	303.07

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C506774&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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1763

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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