Chloromethyl cyanide

Other names:	2-Chloroacetonitrile
	Acetonitrile, 2-chloro-
	Acetonitrile, chloro-
	CH2ClCN
	Chloracetonitrile
	Chloroacetonitrile
	Chloroethanenitrile
	Monochloroacetonitrile
	Monochloromethyl cyanide
	NSC 6180
	UN 2668
	USAF KF-5
	«alpha»-Chloroacetonitrile
	Â«alphaÂ»-Chloroacetonitrile
Inchi:	InChI=1S/C2H2ClN/c3-1-2-4/h1H2
InchiKey:	RENMDAKOXSCIGH-UHFFFAOYSA-N
Formula:	C2H2ClN
SMILES:	N#CCCl
Mol. weight [g/mol]:	75.50
CAS:	107-14-2

Physical Properties

Property code	Value	Unit	Source
affp	745.70	kJ/mol	NIST Webbook
basg	715.10	kJ/mol	NIST Webbook
gf	87.21	kJ/mol	Joback Method
hf	64.53	kJ/mol	Joback Method
hfus	6.64	kJ/mol	Joback Method
hvap	34.91	kJ/mol	Joback Method
ie	11.98	eV	NIST Webbook
ie	12.05	eV	NIST Webbook
ie	11.95 ± 0.01	eV	NIST Webbook
log10ws	-0.09		Estimated Solubility Method
log10ws	-0.09		Aqueous Solubility Prediction Method
logp	0.749		Crippen Method

mcvol	52.660	ml/mol	McGowan Method
pc	4615.13	kPa	Joback Method
rinpol	606.00		NIST Webbook
tb	398.20	K	NIST Webbook
tb	399.70	K	NIST Webbook
tc	588.19	K	Joback Method
tf	207.21	K	Joback Method
vc	0.223	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	72.91	J/mol×K	384.67	Joback Method
cpg	75.72	J/mol×K	418.59	Joback Method
cpg	78.41	J/mol×K	452.51	Joback Method
cpg	80.98	J/mol×K	486.43	Joback Method
cpg	83.43	J/mol×K	520.35	Joback Method
cpg	85.76	J/mol×K	554.27	Joback Method
cpg	87.98	J/mol×K	588.19	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C107142&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume