Propanenitrile, 3-chloro-

Other names:	1-Chloro-2-cyanoethane
	3-Chloropropanenitrile
	3-Chloropropanonitrile
	3-Chloropropionitrile
	3-Chlorpropannitril
	3-chloroprop-2-ynenitrile
	3-chloropropiononitrile
	CH2ClCH2CN
	Cl(CH2)2CN
	NSC 2588
	Propionitrile, 3-chloro-
	Rcra waste number P027
	USAF A-8798
	«beta»-Chloropropionitrile
	Â«betaÂ»-Chloropropionitrile
Inchi:	InChI=1S/C3H4ClN/c4-2-1-3-5/h1-2H2
InchiKey:	GNHMRTZZNHZDDM-UHFFFAOYSA-N
Formula:	C3H4ClN
SMILES:	N#CCCCl
Mol. weight [g/mol]:	89.52
CAS:	542-76-7

Physical Properties

Property code	Value	Unit	Source
affp	773.10	kJ/mol	NIST Webbook
basg	742.40	kJ/mol	NIST Webbook
gf	95.63	kJ/mol	Joback Method
hf	43.89	kJ/mol	Joback Method
hfus	9.23	kJ/mol	Joback Method
hvap	37.14	kJ/mol	Joback Method
log10ws	-0.29		Estimated Solubility Method
log10ws	-0.29		Aqueous Solubility Prediction Method
logp	1.139		Crippen Method
mcvol	66.750	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method

tb	448.70	K	NIST Webbook
tc	609.29	K	Joback Method
tf	222.48	K	Aqueous Solubility Prediction Method
tf	221.70 ± 0.10	K	NIST Webbook
tf	221.63 ± 0.20	K	NIST Webbook
vc	0.279	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	104.40	J/mol×K	407.55	Joback Method
cpg	108.97	J/mol×K	441.17	Joback Method
cpg	113.32	J/mol×K	474.80	Joback Method
cpg	117.47	J/mol×K	508.42	Joback Method
cpg	121.43	J/mol×K	542.05	Joback Method
cpg	125.19	J/mol×K	575.67	Joback Method
cpg	128.77	J/mol×K	609.29	Joback Method

Sources

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
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=C542767&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume