Butanenitrile, 4-chloro-

Other names:	Butyronitrile, 4-chloro-
	«gamma»-Chlorobutyronitrile
	4-Chlorobutanenitrile
	4-Chlorobutyronitrile
Inchi:	InChI=1S/C4H6ClN/c5-3-1-2-4-6/h1-3H2
InchiKey:	ZFCFBWSVQWGOJJ-UHFFFAOYSA-N
Formula:	C4H6ClN
SMILES:	N#CCCCCl
Mol. weight [g/mol]:	103.55
CAS:	628-20-6

Physical Properties

Property code	Value	Unit	Source
gf	104.05	kJ/mol	Joback Method
hf	23.25	kJ/mol	Joback Method
hfus	11.82	kJ/mol	Joback Method
hvap	39.36	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.529		Crippen Method
mcvol	80.840	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
rinpol	862.00		NIST Webbook
rinpol	862.00		NIST Webbook
tb	469.20	K	NIST Webbook
tc	630.14	K	Joback Method
tf	229.75	K	Joback Method
vc	0.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.38	J/mol×K	430.43	Joback Method
cpg	144.54	J/mol×K	463.72	Joback Method
cpg	150.41	J/mol×K	497.00	Joback Method

cpg	156.01	J/mol×K	530.29	Joback Method
cpg	161.34	J/mol×K	563.57	Joback Method
cpg	166.41	J/mol×K	596.86	Joback Method
cpg	171.23	J/mol×K	630.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C628206&Units=SI
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

Legend

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume