Benzonitrile, 4-chloro-

Other names:	Benzonitrile, p-chloro-
	p-Chlorobenzonitrile
	p-Cyanochlorobenzene
	4-Chlorobenzonitrile
	Nitril kyseliny p-chlorbenzoove
	p-Chlorocyanobenzene
	4-Chlorobenzoic acid nitrile
Inchi:	InChI=1S/C7H4ClN/c8-7-3-1-6(5-9)2-4-7/h1-4H
InchiKey:	GJNGXPDXRVXSEH-UHFFFAOYSA-N
Formula:	C7H4ClN
SMILES:	N#Cc1ccc(Cl)cc1
Mol. weight [g/mol]:	137.57
CAS:	623-03-0

Physical Properties

Property code	Value	Unit	Source
gf	232.09	kJ/mol	Joback Method
hf	186.39	kJ/mol	Joback Method
hfus	13.24	kJ/mol	Joback Method
hvap	48.98	kJ/mol	Joback Method
ie	9.94 ± 0.05	eV	NIST Webbook
log10ws	-2.51		Crippen Method
logp	2.212		Crippen Method
mcvol	99.350	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
tb	496.20	K	NIST Webbook
tc	773.11	K	Joback Method
tf	302.50	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.11	J/mol×K	530.73	Joback Method

cpg	189.13	J/mol×K	571.13	Joback Method
cpg	196.55	J/mol×K	611.52	Joback Method
cpg	203.42	J/mol×K	651.92	Joback Method
cpg	209.75	J/mol×K	692.32	Joback Method
cpg	215.58	J/mol×K	732.72	Joback Method
cpg	220.94	J/mol×K	773.11	Joback Method
hvapt	51.90	kJ/mol	436.00	NIST Webbook

Sources

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=C623030&Units=SI

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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