Benzonitrile, 5-chloro-2-nitro-

Other names:	3-Chloro-6-nitrobenzonitrile
	5-Chloro-2-nitrobenzonitrile
	2-Nitro-5-chlorobenzonitrile
Inchi:	InChI=1S/C7H3ClN2O2/c8-6-1-2-7(10(11)12)5(3-6)4-9/h1-3H
InchiKey:	HPWJUEZFOUOUEO-UHFFFAOYSA-N
Formula:	C7H3ClN2O2
SMILES:	N#Cc1cc(Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]:	182.56
CAS:	34662-31-2

Physical Properties

Property code	Value	Unit	Source
gf	258.01	kJ/mol	Joback Method
hf	164.16	kJ/mol	Joback Method
hfus	24.21	kJ/mol	Joback Method
hvap	66.23	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.120		Crippen Method
mcvol	116.770	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	687.55	K	Joback Method
tc	954.98	K	Joback Method
tf	458.63	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.20	J/mol×K	687.55	Joback Method
cpg	256.38	J/mol×K	732.12	Joback Method
cpg	262.90	J/mol×K	776.69	Joback Method
cpg	268.79	J/mol×K	821.27	Joback Method
cpg	274.08	J/mol×K	865.84	Joback Method
cpg	278.83	J/mol×K	910.41	Joback Method

cpg	283.06	J/mol×K	954.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34662312&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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