

2-Propenenitrile, 2-chloro-

Other names:	Acrylonitrile, 2-chloro- «alpha»-Chloroacrylonitrile Chloroacrylonitrile 2-Chloroacrylonitrile Alpha-chloro acrylonitrile Propenenitrile, 2-chloro-
Inchi:	InChI=1S/C3H2CIN/c1-3(4)2-5/h1H2
InchiKey:	OYUNTGBISCIYPW-UHFFFAOYSA-N
Formula:	C3H2CIN
SMILES:	C=C(Cl)C#N
Mol. weight [g/mol]:	87.51
CAS:	920-37-6

Physical Properties

Property code	Value	Unit	Source
ea	4.50	eV	NIST Webbook
gf	174.92	kJ/mol	Joback Method
hf	159.53	kJ/mol	Joback Method
hfus	6.64	kJ/mol	Joback Method
hvap	36.55	kJ/mol	Joback Method
ie	10.58 ± 0.05	eV	NIST Webbook
log10ws	-1.45		Crippen Method
logp	1.262		Crippen Method
mcvol	62.450	ml/mol	McGowan Method
pc	4322.57	kPa	Joback Method
tb	361.70	K	NIST Webbook
tc	614.82	K	Joback Method
tf	202.76	K	Joback Method
vc	0.261	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	90.27	J/mol×K	404.11	Joback Method

cpg	93.96	J/mol×K	439.23	Joback Method
cpg	97.43	J/mol×K	474.35	Joback Method
cpg	100.67	J/mol×K	509.46	Joback Method
cpg	103.72	J/mol×K	544.58	Joback Method
cpg	106.57	J/mol×K	579.70	Joback Method
cpg	109.24	J/mol×K	614.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C920376&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ea:	Electron affinity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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