2-Propenenitrile, 3-chloro-2-methyl-

Other names: 3-chloromethacrylonitrile
Inchi: InChI=1S/C4H4ClN/c1-4(2-5)3-6/h2H,1H3/b4-2+
InchiKey: SRNADAWHRWZEFE-DUXPYHPUSA-N
Formula: C4H4ClN
SMILES: CC(C#N)=CCl
Mol. weight [g/mol]: 101.53
CAS: 10329-37-0

Physical Properties

Property code	Value	Unit	Source
gf	175.72	kJ/mol	Joback Method
hf	130.68	kJ/mol	Joback Method
hfus	10.71	kJ/mol	Joback Method
hvap	39.40	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.653		Crippen Method
mcvol	76.540	ml/mol	McGowan Method
pc	3872.29	kPa	Joback Method
tb	434.47	K	Joback Method
tc	648.87	K	Joback Method
tf	210.71	K	Joback Method
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	121.71	J/mol×K	434.47	Joback Method
cpg	127.28	J/mol×K	470.20	Joback Method
cpg	132.48	J/mol×K	505.94	Joback Method
cpg	137.34	J/mol×K	541.67	Joback Method
cpg	141.87	J/mol×K	577.40	Joback Method
cpg	146.11	J/mol×K	613.14	Joback Method
cpg	150.08	J/mol×K	648.87	Joback Method

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=C10329370&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
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