

3-Chloro-2-methylpropionitrile

Inchi:	InChI=1S/C4H6ClN/c1-4(2-5)3-6/h4H,2H2,1H3
InchiKey:	XXZVBSPSFVERCB-UHFFFAOYSA-N
Formula:	C4H6ClN
SMILES:	CC(C#N)CCl
Mol. weight [g/mol]:	103.55
CAS:	7659-45-2

Physical Properties

Property code	Value	Unit	Source
gf	101.61	kJ/mol	Joback Method
hf	17.97	kJ/mol	Joback Method
hfus	8.30	kJ/mol	Joback Method
hvap	38.97	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.385		Crippen Method
mcvol	80.840	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
tb	429.99	K	Joback Method
tc	634.51	K	Joback Method
tf	214.75	K	Joback Method
vc	0.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.53	J/mol×K	429.99	Joback Method
cpg	144.93	J/mol×K	464.08	Joback Method
cpg	151.03	J/mol×K	498.16	Joback Method
cpg	156.82	J/mol×K	532.25	Joback Method
cpg	162.33	J/mol×K	566.33	Joback Method
cpg	167.55	J/mol×K	600.42	Joback Method
cpg	172.50	J/mol×K	634.51	Joback Method

Sources

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=C7659452&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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