2-CHLOROPROPIONITRILE

Other names: 2-Chloropropionitrile
Propanenitrile, 2-chloro-
Inchi: InChI=1S/C3H4ClN/c1-3(4)2-5/h3H,1H3
InchiKey: JNAYPRPPXRWGQO-UHFFFAOYSA-N
Formula: C3H4ClN
SMILES: CC(Cl)C#N
Mol. weight [g/mol]: 89.52

Physical Properties

Property code	Value	Unit	Source
af	0.3259		Cheméo Relay (1.0)
gf	93.19	kJ/mol	Joback Method
hf	9.51	kJ/mol	Cheméo Relay (1.0)
hfus	5.71	kJ/mol	Joback Method
hvap	44.28	kJ/mol	Cheméo Relay (1.0)
ie	11.75	eV	Cheméo Relay (1.0)
log10ws	-0.55		Cheméo Relay (1.0)
logp	1.137		Crippen Method
mcvol	66.750	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
tb	393.44	K	Cheméo Relay (1.0)
tc	551.90	K	Cheméo Relay (1.0)
tf	236.96	K	Cheméo Relay (1.0)
vc	0.254	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	104.50	J/mol×K	407.11	Joback Method
cpg	109.28	J/mol×K	441.56	Joback Method
cpg	113.83	J/mol×K	476.02	Joback Method
cpg	118.16	J/mol×K	510.47	Joback Method
cpg	122.27	J/mol×K	544.93	Joback Method
cpg	126.17	J/mol×K	579.38	Joback Method

cpg	129.87	J/mol×K	613.84	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1617170&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
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