2,3-Dichloropropionitrile

Other names:	Propanenitrile, 2,3-dichloro- Alpha,beta-dichloropropionitrile 2,3-dichloropropiononitrile
Inchi:	InChI=1S/C3H3Cl2N/c4-1-3(5)2-6/h3H,1H2
InchiKey:	RJJDLPQZNANQDQ-UHFFFAOYSA-N
Formula:	C3H3Cl2N
SMILES:	N#CC(Cl)CCl
Mol. weight [g/mol]:	123.97
CAS:	2601-89-0

Physical Properties

Property code	Value	Unit	Source
gf	81.26	kJ/mol	Joback Method
hf	22.87	kJ/mol	Joback Method
hfus	9.90	kJ/mol	Joback Method
hvap	41.13	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.356		Crippen Method
mcvol	78.990	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
tb	444.54	K	Joback Method
tc	658.60	K	Joback Method
tf	233.40	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	122.35	J/mol×K	444.54	Joback Method
cpg	126.81	J/mol×K	480.22	Joback Method
cpg	131.02	J/mol×K	515.89	Joback Method
cpg	134.97	J/mol×K	551.57	Joback Method
cpg	138.69	J/mol×K	587.25	Joback Method
cpg	142.19	J/mol×K	622.92	Joback Method

cpg	145.46	J/mol×K	658.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2601890&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

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