Acetonitrile, dichloro-

Other names:	Dichloroacetonitrile
	Dichloromethyl cyanide
Inchi:	InChI=1S/C2HCl2N/c3-2(4)1-5/h2H
InchiKey:	STZZWJCGRKXEFF-UHFFFAOYSA-N
Formula:	C2HCl2N
SMILES:	N#CC(Cl)Cl
Mol. weight [g/mol]:	109.94
CAS:	3018-12-0

Physical Properties

Property code	Value	Unit	Source
gf	72.84	kJ/mol	Joback Method
hf	43.51	kJ/mol	Joback Method
hfus	7.31	kJ/mol	Joback Method
hvap	38.91	kJ/mol	Joback Method
ie	12.00	eV	NIST Webbook
ie	12.21	eV	NIST Webbook
log10ws	-1.44		Crippen Method
logp	1.314		Crippen Method
mcvol	64.900	ml/mol	McGowan Method
pc	4438.52	kPa	Joback Method
rinpol	668.00		NIST Webbook
rinpol	693.00		NIST Webbook
tb	385.70	K	NIST Webbook
tc	638.51	K	Joback Method
tf	222.13	K	Joback Method
vc	0.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	88.98	J/mol×K	421.66	Joback Method
cpg	91.71	J/mol×K	457.80	Joback Method
cpg	94.28	J/mol×K	493.94	Joback Method

cpg	96.68	J/mol×K	530.08	Joback Method
cpg	98.93	J/mol×K	566.22	Joback Method
cpg	101.02	J/mol×K	602.36	Joback Method
cpg	102.97	J/mol×K	638.51	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=C3018120&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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume