Cyanogen

Other names:	(CN)2
	CARBON NITRILE
	Carbon nitride
	Carbon nitride (C2N2)
	Cyanogen (C2N2)
	Cyanogen gas
	Cyanogene
	Dicyan
	Dicyanogen
	ETHANEDINITRILE
	NCCN
	Nitriloacetonitrile
	OXALONITRILE
	Oxalic acid dinitrile
	Oxalic nitrile
	Oxalyl cyanide
	Prussite
	Rcra waste number P031
	UN 1026
Inchi:	InChI=1S/C2N2/c3-1-2-4
InchiKey:	JMANVNJQNLATNU-UHFFFAOYSA-N
Formula:	C2N2
SMILES:	N#CC#N
Mol. weight [g/mol]:	52.03
CAS:	460-19-5

Physical Properties

Property code	Value	Unit	Source
af	0.2780		KDB
affp	674.70	kJ/mol	NIST Webbook
basg	621.70	kJ/mol	NIST Webbook
basg	645.80	kJ/mol	NIST Webbook
basg	642.00	kJ/mol	NIST Webbook
basg	622.80	kJ/mol	NIST Webbook
chg	-1096.00 ± 1.80	kJ/mol	NIST Webbook
chg	-1093.70 ± 0.84	kJ/mol	NIST Webbook
chg	-1051.90 ± 5.00	kJ/mol	NIST Webbook

dm	0.20	debye	KDB
gf	297.40	kJ/mol	KDB
hf	309.20	kJ/mol	KDB
hf	308.90 ± 1.80	kJ/mol	NIST Webbook
hf	263.00	kJ/mol	NIST Webbook
hf	306.70 ± 0.84	kJ/mol	NIST Webbook
hfus	3.95	kJ/mol	Joback Method
hvap	20.80	kJ/mol	NIST Webbook
ie	13.50	eV	NIST Webbook
ie	13.37 ± 0.01	eV	NIST Webbook
ie	13.50 ± 0.30	eV	NIST Webbook
ie	13.51	eV	NIST Webbook
ie	13.37 ± 0.01	eV	NIST Webbook
ie	13.36 ± 0.01	eV	NIST Webbook
log10ws	-0.39		Crippen Method
logp	0.034		Crippen Method
mcvol	41.800	ml/mol	McGowan Method
pc	5980.00	kPa	KDB
pt	75.10 ± 1.33	kPa	NIST Webbook
rinpol	273.00		NIST Webbook
rinpol	259.20		NIST Webbook
rinpol	259.20		NIST Webbook
sl	138.83	J/mol×K	NIST Webbook
tb	252.00	K	NIST Webbook
tb	252.00	K	NIST Webbook
tb	252.00	K	KDB
tc	400.00	K	KDB
tf	245.20	K	KDB
tt	245.32 ± 0.02	K	NIST Webbook
vc	0.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	58.91	J/mol×K	449.32	Joback Method
cpg	61.94	J/mol×K	523.13	Joback Method
cpg	63.36	J/mol×K	560.03	Joback Method
cpg	67.25	J/mol×K	670.74	Joback Method
cpg	66.02	J/mol×K	633.84	Joback Method
cpg	64.72	J/mol×K	596.93	Joback Method
cpg	60.46	J/mol×K	486.22	Joback Method

cpl	105.73	J/mol×K	255.00	NIST Webbook
hfust	8.11	kJ/mol	245.32	NIST Webbook
hfust	8.11	kJ/mol	245.30	NIST Webbook
hsubt	32.40	kJ/mol	219.00	NIST Webbook
hsubt	34.40	kJ/mol	223.50	NIST Webbook
hsubt	33.00	kJ/mol	220.50	NIST Webbook
hsubt	33.60	kJ/mol	203.50	NIST Webbook
hvapt	23.30 ± 0.20	kJ/mol	251.95	NIST Webbook
hvapt	23.50	kJ/mol	259.50	NIST Webbook
hvapt	23.90	kJ/mol	259.50	NIST Webbook
hvapt	24.50	kJ/mol	246.50	NIST Webbook
hvapt	23.33	kJ/mol	252.00	NIST Webbook
hvapt	23.33	kJ/mol	252.00	NIST Webbook
rhol	954.00	kg/m3	252.00	KDB
sfust	33.05	J/mol×K	245.32	NIST Webbook
srf	0.02	N/m	217.00	KDB
svapt	92.58	J/mol×K	252.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39745e+01
Coeff. B	-1.79426e+03
Coeff. C	-6.02280e+01
Temperature range (K), min.	191.32
Temperature range (K), max.	400.15

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1412

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C460195&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pt:	Triple Point Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume