Hydrogen cyanide

Other names:	AC
	Acide cyanhydrique
	Acido cianidrico
	Aero Liquid HCN
	Agent AC
	Blausaeure
	Blausaeure (German)
	Blauwzuur
	CARBON HYDRIDE NITIDE
	Carbon hydride nitride
	Carbon hydride nitride (CHN)
	Cyaanwaterstof
	Cyanwasserstoff
	Cyclon
	Cyclone B
	Cyjanowodor
	Evercyn
	FORMONITRILE
	Formic anammonide
	HCN
	HYDROCYANIC ACID
	NA 1051
	Nitrilomethane
	Prussic Acid
	Prussic acid, unstabilized
	Rcra waste number P063
	UN 1051
	Zaclondiscoids
	Zootic acid
Inchi:	InChI=1S/CHN/c1-2/h1H
InchiKey:	LELOWRISYMNNSU-UHFFFAOYSA-N
Formula:	CHN
SMILES:	C#N
Mol. weight [g/mol]:	27.03
CAS:	74-90-8

Physical Properties

Property code	Value	Unit	Source
af	0.3880		KDB
affp	712.90	kJ/mol	NIST Webbook
basg	681.60	kJ/mol	NIST Webbook
dm	3.00	debye	KDB
ea	1.00	eV	NIST Webbook
ea	0.00	eV	NIST Webbook
gf	120.20	kJ/mol	KDB
hf	130.60	kJ/mol	KDB
hfus	1.53	kJ/mol	Joback Method
hvap	28.15	kJ/mol	Joback Method
ie	13.70 ± 0.10	eV	NIST Webbook
ie	13.60 ± 0.01	eV	NIST Webbook
ie	13.59 ± 0.01	eV	NIST Webbook
ie	13.71	eV	NIST Webbook
ie	13.73 ± 0.09	eV	NIST Webbook
ie	13.61	eV	NIST Webbook
ie	13.61 ± 0.00	eV	NIST Webbook
ie	13.60	eV	NIST Webbook
ie	13.60 ± 0.01	eV	NIST Webbook
ie	13.61 ± 0.01	eV	NIST Webbook
log10ws	-0.11		Crippen Method
logp	0.140		Crippen Method
mcvol	26.330	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=4)		KDB
nfpas	%!d(float64=2)		KDB
pc	5390.00	kPa	KDB
rinpol	319.90		NIST Webbook
rinpol	300.00		NIST Webbook
rinpol	319.90		NIST Webbook
rinpol	320.00		NIST Webbook
sl	113.01	J/mol×K	NIST Webbook
tb	298.90 ± 0.50	K	NIST Webbook
tb	299.00 ± 1.50	K	NIST Webbook
tb	299.00	K	KDB
tb	299.00 ± 0.40	K	NIST Webbook
tb	298.90 ± 0.40	K	NIST Webbook
tb	299.40 ± 0.60	K	NIST Webbook
tb	298.90 ± 0.50	K	NIST Webbook
tb	298.90 ± 0.50	K	NIST Webbook
tb	298.90 ± 0.50	K	NIST Webbook
tb	299.08 ± 0.40	K	NIST Webbook
tb	299.70 ± 0.50	K	NIST Webbook

tb	298.90 ± 1.00	K	NIST Webbook
tb	299.50 ± 1.00	K	NIST Webbook
tb	298.90 ± 0.40	K	NIST Webbook
tb	298.90 ± 0.30	K	NIST Webbook
tb	298.80 ± 0.50	K	NIST Webbook
tc	456.70	K	KDB
tf	259.20 ± 0.50	K	NIST Webbook
tf	259.88 ± 0.10	K	NIST Webbook
tf	259.86 ± 0.05	K	NIST Webbook
tf	259.70	K	KDB
tf	259.75 ± 0.50	K	NIST Webbook
tf	259.81 ± 0.50	K	NIST Webbook
tf	259.85 ± 0.30	K	NIST Webbook
tf	258.30 ± 1.00	K	NIST Webbook
tf	259.80 ± 0.20	K	NIST Webbook
tf	259.75 ± 0.30	K	NIST Webbook
tf	258.29 ± 1.00	K	NIST Webbook
tf	259.00 ± 1.50	K	NIST Webbook
tf	259.85 ± 0.20	K	NIST Webbook
tf	286.50 ± 0.20	K	NIST Webbook
tf	259.90 ± 0.10	K	NIST Webbook
tt	259.86 ± 0.02	K	NIST Webbook
vc	0.139	m3/kmol	KDB
zc	0.1973040		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	24.62	J/mol×K	323.66	Joback Method
cpg	25.63	J/mol×K	355.42	Joback Method
cpg	26.44	J/mol×K	387.18	Joback Method
cpg	27.08	J/mol×K	418.95	Joback Method
cpg	27.56	J/mol×K	450.71	Joback Method
cpg	27.91	J/mol×K	482.47	Joback Method
cpg	28.13	J/mol×K	514.23	Joback Method
cpl	71.00	J/mol×K	300.00	NIST Webbook
hfust	8.41	kJ/mol	259.90	NIST Webbook
hsubt	35.60	kJ/mol	247.50	NIST Webbook
hsubt	37.60	kJ/mol	228.00	NIST Webbook
hvapt	25.22	kJ/mol	298.85	NIST Webbook
hvapt	28.10	kJ/mol	279.00	NIST Webbook

hvapt	27.80	kJ/mol	377.50	NIST Webbook
hvapt	28.10	kJ/mol	286.00	NIST Webbook
hvapt	28.00	kJ/mol	276.50	NIST Webbook
hvapt	27.80	kJ/mol	282.50	NIST Webbook
hvapt	28.10	kJ/mol	288.00	NIST Webbook
hvapt	27.20	kJ/mol	287.50	NIST Webbook
rhol	688.00	kg/m3	293.00	KDB
sfust	32.34	J/mol×K	259.90	NIST Webbook
svapt	84.38	J/mol×K	298.85	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64196e+01
Coeff. B	-3.69077e+03
Coeff. C	1.37430e+01
Temperature range (K), min.	215.04
Temperature range (K), max.	456.65

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1940
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74908&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
ea:	Electron affinity
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical 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
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
zc:	Critical Compressibility