2-Propenenitrile

Other names:	Acritet
	Acrylnitril
	Acrylon
	Acrylonitrile
	Acrylonitrile monomer
	Akrylonitril
	Akrylonitryl
	CH2CHCN
	Carbacryl
	Cianuro di vinile
	Cyanoethene
	Cyanoethylene
	Cyanure de vinyle
	ENT 54
	Fumigrain
	Miller's fumigrain
	NSC 6362
	Nitrile acrilico
	Nitrile acrylique
	Propenenitrile
	Propenitrile
	Propenonitrile
	Rcra waste number U009
	TL 314
	UN 1093
	VCN
	Ventox
	Vinyl cyanide
	Vinylkyanid
Inchi:	InChI=1S/C3H3N/c1-2-3-4/h2H,1H2
InchiKey:	NLHHRLWOUZZQLW-UHFFFAOYSA-N
Formula:	C3H3N
SMILES:	C=CC#N
Mol. weight [g/mol]:	53.06
CAS:	107-13-1

Physical Properties

Property code	Value	Unit	Source
af	0.3500		KDB
affp	784.70	kJ/mol	NIST Webbook
aigt	754.26	K	KDB
basg	753.70	kJ/mol	NIST Webbook
chl	-1759.00 ± 3.00	kJ/mol	NIST Webbook
chl	-1756.40 ± 0.42	kJ/mol	NIST Webbook
dm	3.50	debye	KDB
ea	0.01	eV	NIST Webbook
ea	0.01	eV	NIST Webbook
fll	3.05	% in Air	KDB
flu	17.00	% in Air	KDB
fpc	272.59	K	KDB
fpo	272.04	K	KDB
gf	195.40	kJ/mol	KDB
gyrad	2.4430		KDB
hf	179.70	kJ/mol	NIST Webbook
hf	172.60	kJ/mol	NIST Webbook
hf	185.10	kJ/mol	KDB
hfl	147.10	kJ/mol	NIST Webbook
hfl	140.00	kJ/mol	NIST Webbook
hfus	3.75	kJ/mol	Joback Method
hvap	33.00	kJ/mol	NIST Webbook
hvap	32.60	kJ/mol	NIST Webbook
hvap	33.00	kJ/mol	NIST Webbook
hvap	31.60	kJ/mol	NIST Webbook
ie	10.92 ± 0.05	eV	NIST Webbook
ie	10.91 ± 0.01	eV	NIST Webbook
ie	10.91	eV	NIST Webbook
ie	10.91	eV	NIST Webbook
ie	10.91	eV	NIST Webbook
ie	10.91 ± 0.01	eV	NIST Webbook
ie	11.10	eV	NIST Webbook
log10ws	0.15		Aqueous Solubility Prediction Method
log10ws	0.15		Estimated Solubility Method
logp	0.696		Crippen Method
mcvol	50.210	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=4)		KDB
nfpas	%!d(float64=2)		KDB
pc	4560.00	kPa	KDB
pc	4660.00 ± 20.00	kPa	NIST Webbook

rinpol	492.00		NIST Webbook
rinpol	521.10		NIST Webbook
rinpol	495.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	491.00		NIST Webbook
rinpol	488.00		NIST Webbook
rinpol	516.00		NIST Webbook
rinpol	495.00		NIST Webbook
rinpol	490.00		NIST Webbook
rinpol	516.00		NIST Webbook
rinpol	482.00		NIST Webbook
rinpol	492.00		NIST Webbook
rinpol	520.00		NIST Webbook
rinpol	521.10		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	540.00		NIST Webbook
rinpol	476.00		NIST Webbook
rinpol	496.40		NIST Webbook
rinpol	544.00		NIST Webbook
rinpol	482.00		NIST Webbook
rinpol	495.00		NIST Webbook
ripol	1010.00		NIST Webbook
ripol	993.00		NIST Webbook
sl	178.91	J/mol×K	NIST Webbook
tb	350.50	K	KDB
tc	536.00	K	KDB
tc	540.00 ± 2.00	K	NIST Webbook
tf	189.60 ± 0.10	K	NIST Webbook
tf	189.47 ± 0.20	K	NIST Webbook
tf	189.55	K	NIST Webbook
tf	191.00 ± 2.00	K	NIST Webbook
tf	189.50	K	KDB
tf	189.40	K	Aqueous Solubility Prediction Method
tt	189.63	K	KDB
tt	189.63 ± 0.01	K	NIST Webbook
vc	0.210	m3/kmol	KDB
zc	0.2148730		KDB
zra	0.23		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	76.85	J/mol×K	399.75	Joback Method
cpg	93.67	J/mol×K	564.51	Joback Method
cpg	90.64	J/mol×K	531.56	Joback Method
cpg	87.46	J/mol×K	498.60	Joback Method
cpg	84.10	J/mol×K	465.65	Joback Method
cpg	80.57	J/mol×K	432.70	Joback Method
cpg	72.94	J/mol×K	366.80	Joback Method
cpl	113.00	J/mol×K	298.00	NIST Webbook
cpl	106.70	J/mol×K	297.00	NIST Webbook
cpl	108.78	J/mol×K	298.15	NIST Webbook
cpl	98.70	J/mol×K	298.15	NIST Webbook
dvisc	0.0003440	Pa×s	298.15	Density and Viscosity of Acrylonitrile + Cinnamaldehyde, + Anisaldehyde, and + Benzaldehyde at (298.15, 308.15, and 318.15) K
dvisc	0.0003070	Pa×s	308.15	Density and Viscosity of Acrylonitrile + Cinnamaldehyde, + Anisaldehyde, and + Benzaldehyde at (298.15, 308.15, and 318.15) K
dvisc	0.0002840	Pa×s	318.15	Density and Viscosity of Acrylonitrile + Cinnamaldehyde, + Anisaldehyde, and + Benzaldehyde at (298.15, 308.15, and 318.15) K
hfust	6.23	kJ/mol	189.60	NIST Webbook
hfust	1.19	kJ/mol	162.50	NIST Webbook
hfust	6.23	kJ/mol	189.60	NIST Webbook
hvapt	32.90	kJ/mol	318.00	NIST Webbook
hvapt	35.50	kJ/mol	286.50	NIST Webbook
hvapt	32.63	kJ/mol	350.50	KDB
hvapt	33.60	kJ/mol	304.50	NIST Webbook
hvapt	32.60	kJ/mol	313.00	NIST Webbook
pvap	95.50	kPa	348.75	Vapor-liquid equilibrium and excess Gibbs energies of some binary mixtures of acrylonitrile at 95.5 kPa

rfi	1.39080		293.15	Liquid liquid equilibrium for the ternary systems of water + methanol + acrylonitrile
rfi	1.38880		298.15	Bubble temperature measurements on seven binary mixtures formed by ethylbenzene at 94.7 kPa
rfi	1.38880		298.15	Activity coefficients in binary mixtures formed by cyclohexanone with a variety of compounds at 94.7 kPa
rhol	806.00	kg/m3	293.15	Isobaric Vapor Liquid Equilibrium Data of Acrylonitrile (1) + Heptan-1-ol (2), Acrylonitrile (1) + Ethanol (2), and Nitrobenzene (1) + Heptan-1-ol (2) at 96.5 kPa
rhol	800.30	kg/m3	298.15	Bubble point measurements of binary mixtures formed by 1-hexanol with selected nitro-compounds and substituted benzenes at 95.6 kPa
rhol	806.00	kg/m3	293.00	KDB
sfust	7.32	J/mol×K	162.50	NIST Webbook
sfust	32.84	J/mol×K	189.60	NIST Webbook
srf	0.03	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50433e+01
Coeff. B	-3.40158e+03

Coeff. C	-2.47100e+01
Temperature range (K), min.	255.24
Temperature range (K), max.	374.24

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.37047e+01
Coeff. B	-6.15193e+03
Coeff. C	-8.99499e+00
Coeff. D	9.44061e-06
Temperature range (K), min.	189.63
Temperature range (K), max.	535.00

Sources

Activity coefficients in binary mixtures formed by cyclohexanone with a variety of compounds at 94.7 kPa:	https://www.doi.org/10.1016/j.fluid.2005.06.022
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535
Density and Viscosity of Acrylonitrile + Cinnamaldehyde, + Anisaldehyde, and + Benzaldehyde at (298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1021/je7006742
KDB, Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1401
Bubble point measurements of binary mixtures formed by 1-hexanol with selected nitro compounds and substituted benzenes at 95.6 kPa :	https://www.doi.org/10.1016/j.fluid.2010.08.010
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1401
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Bubble temperature measurements on seven binary mixtures formed by ethylbenzene at 94.7 kPa:	https://www.doi.org/10.1016/j.jct.2004.11.015
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107131&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Isobaric Vapor Liquid Equilibrium Data of Acrylonitrile (1) + Heptan-1-ol (2), Acrylonitrile (1) + Ethanol (2), and Chlorobenzene (1) + Heptan-1-ol (2) at 95.3 kPa:	https://www.doi.org/10.1021/je400214b
Liquid-liquid equilibrium for the ternary systems of water + methanol + acrylonitrile:	https://www.doi.org/10.1021/je2009208
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Vapor-liquid equilibrium and excess Gibbs energies of some binary mixtures of acrylonitrile at 95.3 kPa:	https://www.doi.org/10.1016/j.fluid.2008.03.020
Phase Equilibria of Acrylonitrile and p-Bromobenzaldehyde in Carbon Dioxide:	https://www.doi.org/10.1021/je700448v
KDB, Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1401

Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
ea:	Electron affinity
fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
fpc:	Flash Point (Closed Cup Method)
fpo:	Flash Point (Open Cup Method)
gf:	Standard Gibbs free energy of formation
gyrad:	Radius of Gyration
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion 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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter