

Propanenitrile

Other names:	C2H5CN
	CYANOETHANE
	ETHER CYANATUS
	Ethyl cyanide
	Ethylkyanid
	HYDROCYANIC ETHER
	NSC 7966
	PROPIONITRILE
	Propannitril
	Propionic nitrile
	Propiononitrile
	Propylnitrile
	Rcra waste number P101
	UN 2404
	ethanecarbonitrile
	n-Propanenitrile
Inchi:	InChI=1S/C3H5N/c1-2-3-4/h2H2,1H3
InchiKey:	FVSKHRXBFJPNKK-UHFFFAOYSA-N
Formula:	C3H5N
SMILES:	CCC#N
Mol. weight [g/mol]:	55.08
CAS:	107-12-0

Physical Properties

Property code	Value	Unit	Source
af	0.3130		KDB
affp	794.10	kJ/mol	NIST Webbook
basg	763.00	kJ/mol	NIST Webbook
chl	-1918.00	kJ/mol	NIST Webbook
chl	-1948.30 ± 0.54	kJ/mol	NIST Webbook
dm	3.70	debye	KDB
ea	0.02 ± 0.00	eV	NIST Webbook
gf	96.21	kJ/mol	KDB
hf	50.66	kJ/mol	KDB
hf	51.46	kJ/mol	NIST Webbook
hfl	15.50	kJ/mol	NIST Webbook

hfus	5.03	kJ/mol	Joback Method
hvap	36.03 ± 0.02	kJ/mol	NIST Webbook
hvap	36.00	kJ/mol	NIST Webbook
hvap	36.00	kJ/mol	NIST Webbook
hvap	36.70 ± 0.30	kJ/mol	NIST Webbook
hvap	37.10 ± 0.30	kJ/mol	NIST Webbook
hvap	36.19	kJ/mol	NIST Webbook
ie	11.85	eV	NIST Webbook
ie	11.90	eV	NIST Webbook
ie	11.85 ± 0.02	eV	NIST Webbook
ie	11.84 ± 0.02	eV	NIST Webbook
ie	11.85 ± 0.01	eV	NIST Webbook
ie	11.50 ± 0.25	eV	NIST Webbook
log10ws	0.28		Estimated Solubility Method
log10ws	0.28		Aqueous Solubility Prediction Method
logp	0.920		Crippen Method
mccvol	54.510	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=4)		KDB
nfpas	%!d(float64=1)		KDB
pc	4260.00 ± 10.00	kPa	NIST Webbook
pc	4180.00 ± 91.19	kPa	NIST Webbook
pc	4174.59 ± 81.06	kPa	NIST Webbook
pc	4194.85 ± 81.06	kPa	NIST Webbook
pc	4260.00	kPa	KDB
rinpol	545.05		NIST Webbook
rinpol	543.33		NIST Webbook
rinpol	543.83		NIST Webbook
rinpol	544.44		NIST Webbook
rinpol	580.00		NIST Webbook
rinpol	545.79		NIST Webbook
rinpol	546.65		NIST Webbook
rinpol	547.65		NIST Webbook
rinpol	548.60		NIST Webbook
rinpol	549.63		NIST Webbook
rinpol	550.75		NIST Webbook
rinpol	543.13		NIST Webbook
rinpol	542.69		NIST Webbook
rinpol	542.41		NIST Webbook
rinpol	542.29		NIST Webbook
rinpol	554.00		NIST Webbook
rinpol	542.38		NIST Webbook
rinpol	542.60		NIST Webbook

rinpol	542.90		NIST Webbook
rinpol	592.00		NIST Webbook
rinpol	545.30		NIST Webbook
rinpol	523.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	547.00		NIST Webbook
rinpol	533.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	510.00		NIST Webbook
rinpol	573.70		NIST Webbook
rinpol	554.00		NIST Webbook
rinpol	554.00		NIST Webbook
rinpol	555.00		NIST Webbook
rinpol	542.32		NIST Webbook
rinpol	544.00		NIST Webbook
rinpol	557.00		NIST Webbook
rinpol	539.00		NIST Webbook
rinpol	542.00		NIST Webbook
rinpol	539.00		NIST Webbook
rinpol	580.00		NIST Webbook
rinpol	580.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	524.00		NIST Webbook
ripol	1015.00		NIST Webbook
ripol	1046.00		NIST Webbook
ripol	1023.00		NIST Webbook
sl	189.33	J/mol×K	NIST Webbook
tb	371.00 ± 2.00	K	NIST Webbook
tb	371.40 ± 1.00	K	NIST Webbook
tb	391.70 ± 2.00	K	NIST Webbook
tb	370.29	K	KDB
tb	370.50	K	NIST Webbook
tb	371.00	K	NIST Webbook
tb	370.45 ± 0.50	K	NIST Webbook
tb	370.50 ± 0.30	K	NIST Webbook
tb	370.50 ± 0.30	K	NIST Webbook
tb	370.00 ± 1.00	K	NIST Webbook
tb	370.48 ± 0.20	K	NIST Webbook
tb	370.00 ± 1.50	K	NIST Webbook
tb	370.31 ± 0.40	K	NIST Webbook
tb	371.00 ± 1.50	K	NIST Webbook
tb	370.30 ± 0.50	K	NIST Webbook
tb	369.70 ± 2.00	K	NIST Webbook
tb	370.50 ± 0.07	K	NIST Webbook

tb	370.15 ± 1.50	K	NIST Webbook
tb	390.00 ± 3.00	K	NIST Webbook
tb	368.00 ± 2.00	K	NIST Webbook
tb	370.00 ± 2.00	K	NIST Webbook
tb	370.29 ± 0.30	K	NIST Webbook
tb	369.80 ± 0.40	K	NIST Webbook
tb	370.35 ± 0.30	K	NIST Webbook
tb	370.40 ± 0.30	K	NIST Webbook
tb	369.00 ± 2.00	K	NIST Webbook
tb	370.30 ± 0.50	K	NIST Webbook
tb	370.00 ± 0.40	K	NIST Webbook
tb	370.00 ± 2.00	K	NIST Webbook
tb	370.30 ± 0.30	K	NIST Webbook
tb	370.40 ± 0.10	K	NIST Webbook
tb	370.40 ± 0.30	K	NIST Webbook
tb	365.00 ± 5.00	K	NIST Webbook
tb	370.80 ± 0.70	K	NIST Webbook
tb	370.80 ± 0.60	K	NIST Webbook
tb	369.00 ± 1.50	K	NIST Webbook
tc	561.30	K	KDB
tc	558.85 ± 1.00	K	NIST Webbook
tc	558.70 ± 2.00	K	NIST Webbook
tc	561.30 ± 0.20	K	NIST Webbook
tc	558.85 ± 1.00	K	NIST Webbook
tf	180.26	K	KDB
tf	181.25 ± 0.20	K	NIST Webbook
tf	181.30 ± 0.20	K	NIST Webbook
tf	180.59	K	Aqueous Solubility Prediction Method
tf	180.30 ± 0.60	K	NIST Webbook
tf	181.30 ± 0.20	K	NIST Webbook
tf	171.15 ± 6.00	K	NIST Webbook
tf	182.00 ± 2.00	K	NIST Webbook
tf	181.15 ± 0.50	K	NIST Webbook
tf	180.26 ± 0.10	K	NIST Webbook
tt	180.37 ± 0.02	K	NIST Webbook
vc	0.229	m3/kmol	KDB
zc	0.2090320		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	90.77	J/mol×K	402.34	Joback Method
cpg	95.36	J/mol×K	434.56	Joback Method
cpg	99.78	J/mol×K	466.78	Joback Method
cpg	104.02	J/mol×K	499.00	Joback Method
cpg	108.09	J/mol×K	531.23	Joback Method
cpg	112.00	J/mol×K	563.45	Joback Method
cpg	86.00	J/mol×K	370.12	Joback Method
cpl	105.30	J/mol×K	298.15	NIST Webbook
cpl	112.90	J/mol×K	297.00	NIST Webbook
cpl	119.50	J/mol×K	298.15	NIST Webbook
cpl	106.00	J/mol×K	303.15	NIST Webbook
dvisc	0.0003822	Pa×s	308.15	Molecular interaction studies and theoretical estimation of ultrasonic speeds using scaled particle theory in binary mixtures of toluene with homologous nitriles at different temperatures
dvisc	0.0004107	Pa×s	298.15	Molecular interaction studies and theoretical estimation of ultrasonic speeds using scaled particle theory in binary mixtures of toluene with homologous nitriles at different temperatures
dvisc	0.0003991	Pa×s	303.15	Molecular interaction studies and theoretical estimation of ultrasonic speeds using scaled particle theory in binary mixtures of toluene with homologous nitriles at different temperatures
hfust	17.07	kJ/mol	177.00	NIST Webbook
hfust	5.03	kJ/mol	180.40	NIST Webbook
hfust	5.03	kJ/mol	180.40	NIST Webbook
hvapt	31.81	kJ/mol	371.00	NIST Webbook

hvapt	36.12	kJ/mol	298.15	NIST Webbook
hvapt	32.26	kJ/mol	370.30	KDB
hvapt	36.70	kJ/mol	335.50	NIST Webbook
hvapt	35.90	kJ/mol	339.00	NIST Webbook
hvapt	36.50	kJ/mol	242.00	NIST Webbook
hvapt	36.10	kJ/mol	329.50	NIST Webbook
pvap	59.51	kPa	353.63	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile
pvap	84.93	kPa	364.69	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile
pvap	80.76	kPa	363.02	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile
pvap	91.88	kPa	367.21	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile

pvap	69.91	kPa	358.53	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile
pvap	64.72	kPa	356.17	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile
pvap	96.66	kPa	368.88	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile
pvap	54.93	kPa	351.26	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile
pvap	50.91	kPa	349.02	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile

pvap	46.11	kPa	346.17	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile
pvap	37.95	kPa	340.70	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile
pvap	27.73	kPa	332.31	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile
pvap	103.78	kPa	371.23	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile

pvap	18.58	kPa	322.25	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile
pvap	80.66	kPa	363.10	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile
pvap	58.60	kPa	353.15	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol
pvap	49.32	kPa	348.09	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol
pvap	41.33	kPa	343.08	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol
pvap	34.61	kPa	338.22	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol
pvap	31.64	kPa	335.82	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol

pvap	28.57	kPa	333.15	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol
pvap	21.46	kPa	325.79	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile
pvap	26.11	kPa	330.82	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol
pvap	23.64	kPa	328.27	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol
pvap	21.35	kPa	325.74	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol
pvap	19.22	kPa	323.15	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol
pvap	17.22	kPa	320.51	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol
pvap	15.71	kPa	318.35	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol

pvap	14.14	kPa	315.89	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol
pvap	12.55	kPa	313.15	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol
pvap	10.59	kPa	309.38	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol
pvap	69.60	kPa	358.33	Phase equilibrium measurements for systems containing propanenitrile with tert-butyl ethyl ether and C4-hydrocarbons
pvap	17.40	kPa	322.00	Phase equilibrium measurements for systems containing propanenitrile with tert-butyl ethyl ether and C4-hydrocarbons
pvap	12.50	kPa	313.15	Phase equilibrium measurements for systems containing propanenitrile with tert-butyl ethyl ether and C4-hydrocarbons
pvap	11.90	kPa	312.58	Phase equilibrium measurements for systems containing propanenitrile with tert-butyl ethyl ether and C4-hydrocarbons

pvap	11.90	kPa	312.50	Phase equilibrium measurements for systems containing propanenitrile with tert-butyl ethyl ether and C4-hydrocarbons
pvap	11.55	kPa	311.56	Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and 1-Pentanamine + 1-Methoxy-2-propanol
pvap	75.34	kPa	360.86	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing 2-Ethoxy-2-methylpropane or 2-Ethoxy-2-methylbutane and Acetonitrile or Propanenitrile
pvap	9.47	kPa	307.78	Phase equilibrium measurements for systems containing propanenitrile with tert-butyl ethyl ether and C4-hydrocarbons
rfi	1.36330		298.15	Excess molar volumes and partial molar volumes for (propionitrile + an alkanol) at T = 298.15 K and p = 0.1 MPa
rfi	1.36368		298.15	Vapor-Liquid Equilibrium Data for the Binary Methyl Esters (Butyrate, Pentanoate, and Hexanoate) (1) + Propanenitrile (2) Systems at 93.32 kPa

rhoI	777.69	kg/m3	298.15	Calorimetric Study of Nitrile Group-Solvent Interactions and Comparison with Dispersive Quasi-Chemical (DISQUAC) Predictions
rhoI	776.70	kg/m3	298.15	Speed of sound as a function of temperature and pressure for propane derivatives
rhoI	782.00	kg/m3	293.00	KDB
sfust	9.67	J/mol×K	177.00	NIST Webbook
sfust	27.91	J/mol×K	180.40	NIST Webbook
srf	0.03	N/m	298.15	Concentration Dependence of Surface Tension for Very Dilute Aqueous Solutions of Organic Non-Electrolytes
srf	0.03	N/m	293.20	KDB
svapt	121.10	J/mol×K	298.15	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42491e+01
Coeff. B	-2.93590e+03
Coeff. C	-6.51540e+01
Temperature range (K), min.	275.44
Temperature range (K), max.	564.40

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	6.95302e+01
Coeff. B	-6.51183e+03
Coeff. C	-8.13958e+00
Coeff. D	6.11437e-06

Temperature range (K), min.	180.26
Temperature range (K), max.	564.40

Sources

Experimental (Solid + Liquid) and (Liquid + Liquid) Equilibria and Excess Molar Volumes for the Acetonitrile, Propanenitrile and Butanenitrile Mixtures
 The Yaws Handbook of Vapor Pressure:
 Phase equilibrium measurements for systems containing propanenitrile with speed of sound as a function of temperature and pressure for propane derivatives
 Determination of Henry's Law Constants Using Internal Standards
 Vapor-Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes for Binary Mixtures of Nitrile Group Solvent Interactions and Molecular Interactions Studies and Measurements of Henry's Law and Excess Molar Enthalpies and Excess Molar Volumes for Propanenitrile
 Vapor-Liquid Equilibrium for Acetonitrile + Propanenitrile and Ethanol + Propanenitrile
 Joback Method:
 Concentration Dependence of Surface Tension for Very Dilute Aqueous Solutions of Organic Protonic Acids
 McGowan Method:
 Vapor-Liquid Equilibrium Data for the Binary Methyl Esters (Butyrate, Pentanoate, and Hexanoate) and Partial Molar Volumes of Systems at 0.3 and 0.5 MPa at 298.15 K and p = 0.1 MPa:

<https://www.doi.org/10.1021/je050262m>
<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1387>
<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<https://www.doi.org/10.1016/j.fluid.2010.09.023>
<https://www.doi.org/10.1016/j.jct.2016.12.016>
<https://www.doi.org/10.1021/je3010535>
<https://www.doi.org/10.1021/je301238f>
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<https://www.doi.org/10.1016/j.tca.2009.10.001>
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<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1387>
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<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1387>
https://en.wikipedia.org/wiki/Joback_method
<https://www.doi.org/10.1021/je049955d>
<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>
<http://link.springer.com/article/10.1007/BF02311772>
<https://www.doi.org/10.1021/je060469v>
<https://www.doi.org/10.1016/j.jct.2005.05.007>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C107120&Units=SI>

Legend

af: Acentric Factor
 affp: Proton affinity
 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

gf:	Standard Gibbs free energy of formation
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
rhof:	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
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

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