Benzonitrile

Other names:	Benzene, cyano-
	Benzenenitrile
	Benzoic acid nitrile
	Cyanobenzene
	Fenylkyanid
	Phenyl cyanide
	UN 2224
Inchi:	InChI=1S/C7H5N/c8-6-7-4-2-1-3-5-7/h1-5H
InchiKey:	JFDZBHWFFUWGJE-UHFFFAOYSA-N
Formula:	C7H5N
SMILES:	N#Cc1ccccc1
Mol. weight [g/mol]:	103.12
CAS:	100-47-0

Physical Properties

Property code	Value	Unit	Source
af	0.3620		KDB
affp	811.50	kJ/mol	NIST Webbook
basg	780.90	kJ/mol	NIST Webbook
chl	-3632.30 ± 1.50	kJ/mol	NIST Webbook
chl	-3632.30	kJ/mol	NIST Webbook
cpl	166.41	J/mol×K	Thermodynamics of mixtures involving some (benzene derivatives + benzonitrile)
dm	3.50	debye	KDB
ea	0.26 ± 0.02	eV	NIST Webbook
ea	0.26 ± 0.10	eV	NIST Webbook
fpo	348.15	K	KDB
gf	261.00	kJ/mol	KDB
hf	219.00	kJ/mol	KDB
hf	219.00	kJ/mol	NIST Webbook
hf	219.00	kJ/mol	NIST Webbook
hfl	163.20 ± 1.50	kJ/mol	NIST Webbook
hfl	163.20 ± 1.50	kJ/mol	NIST Webbook
hfus	9.43	kJ/mol	Joback Method
hvap	55.48	kJ/mol	NIST Webbook
hvap	55.80	kJ/mol	NIST Webbook

ie	9.73 ± 0.01	eV	NIST Webbook
ie	9.72	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
ie	9.71	eV	NIST Webbook
ie	10.02	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	9.79	eV	NIST Webbook
ie	9.71 ± 0.01	eV	NIST Webbook
ie	9.77	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
ie	9.62	eV	NIST Webbook
ie	9.69	eV	NIST Webbook
ie	10.13 ± 0.03	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
ie	9.73 ± 0.00	eV	NIST Webbook
ie	9.71	eV	NIST Webbook
log10ws	-1.00		Estimated Solubility Method
log10ws	-1.00		Aqueous Solubility Prediction Method
logp	1.558		Crippen Method
mcvol	87.110	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=1)		KDB
nfpas	%!d(float64=1)		KDB
pc	4215.12 ± 151.99	kPa	NIST Webbook
pc	4210.00	kPa	KDB
pc	4220.00 ± 101.32	kPa	NIST Webbook
pc	4215.00 ± 4.00	kPa	NIST Webbook
pc	4215.12 ± 151.99	kPa	NIST Webbook
rhoc	313.18 ± 3.09	kg/m3	NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	150.10		NIST Webbook
rinpol	150.40		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	965.00		NIST Webbook

rinpol	943.00	NIST Webbook
rinpol	992.00	NIST Webbook
rinpol	992.00	NIST Webbook
rinpol	953.00	NIST Webbook
rinpol	936.00	NIST Webbook
rinpol	965.00	NIST Webbook
rinpol	973.00	NIST Webbook
rinpol	994.00	NIST Webbook
rinpol	937.30	NIST Webbook
rinpol	987.90	NIST Webbook
rinpol	986.00	NIST Webbook
rinpol	992.00	NIST Webbook
rinpol	983.40	NIST Webbook
rinpol	976.00	NIST Webbook
rinpol	983.00	NIST Webbook
rinpol	1003.00	NIST Webbook
rinpol	981.00	NIST Webbook
rinpol	956.00	NIST Webbook
rinpol	947.00	NIST Webbook
rinpol	951.00	NIST Webbook
rinpol	954.00	NIST Webbook
rinpol	962.00	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	948.00	NIST Webbook
rinpol	989.00	NIST Webbook
rinpol	989.90	NIST Webbook
rinpol	985.00	NIST Webbook
rinpol	982.00	NIST Webbook
rinpol	993.00	NIST Webbook
rinpol	994.00	NIST Webbook
rinpol	984.00	NIST Webbook
rinpol	984.00	NIST Webbook
rinpol	965.00	NIST Webbook
rinpol	988.00	NIST Webbook
rinpol	951.00	NIST Webbook
rinpol	981.00	NIST Webbook
rinpol	965.00	NIST Webbook
rinpol	940.10	NIST Webbook
ripol	1629.00	NIST Webbook
ripol	1583.00	NIST Webbook
ripol	1583.00	NIST Webbook
ripol	1614.00	NIST Webbook
ripol	1570.00	NIST Webbook
ripol	1591.00	NIST Webbook

ripol	1583.00		NIST Webbook
ripol	1583.00		NIST Webbook
sl	209.10	J/mol×K	NIST Webbook
sl	209.10	J/mol×K	NIST Webbook
sl	209.10	J/mol×K	NIST Webbook
tb	463.85 ± 0.50	K	NIST Webbook
tb	464.30 ± 0.70	K	NIST Webbook
tb	464.00 ± 0.40	K	NIST Webbook
tb	464.10 ± 0.60	K	NIST Webbook
tb	461.90 ± 1.00	K	NIST Webbook
tb	464.50 ± 0.30	K	NIST Webbook
tb	464.15 ± 0.30	K	NIST Webbook
tb	463.80	K	NIST Webbook
tb	464.00	K	NIST Webbook
tb	463.90	K	NIST Webbook
tb	462.70	K	NIST Webbook
tb	464.30	K	KDB
tb	464.45 ± 0.30	K	NIST Webbook
tb	464.25 ± 0.30	K	NIST Webbook
tb	463.85 ± 0.60	K	NIST Webbook
tc	701.25 ± 2.50	K	NIST Webbook
tc	699.20 ± 3.00	K	NIST Webbook
tc	699.40 ± 1.00	K	NIST Webbook
tc	699.40	K	KDB
tc	700.45 ± 2.50	K	NIST Webbook
tc	699.35 ± 2.50	K	NIST Webbook
tc	705.25 ± 2.50	K	NIST Webbook
tf	259.35 ± 0.50	K	NIST Webbook
tf	259.15 ± 0.00	K	NIST Webbook
tf	260.40 ± 0.15	K	NIST Webbook
tf	260.05 ± 0.30	K	NIST Webbook
tf	259.35 ± 0.40	K	NIST Webbook
tf	286.15 ± 1.00	K	NIST Webbook
tf	260.00	K	NIST Webbook
tf	260.40	K	KDB
tf	260.28 ± 0.25	K	NIST Webbook
tf	260.22	K	Aqueous Solubility Prediction Method
tt	260.33 ± 0.02	K	NIST Webbook
tt	260.33 ± 0.02	K	NIST Webbook
tt	260.33 ± 0.02	K	NIST Webbook
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.30	J/mol×K	488.32	Joback Method
cpg	186.79	J/mol×K	606.29	Joback Method
cpg	194.06	J/mol×K	645.62	Joback Method
cpg	200.77	J/mol×K	684.94	Joback Method
cpg	206.96	J/mol×K	724.27	Joback Method
cpg	178.93	J/mol×K	566.97	Joback Method
cpg	170.44	J/mol×K	527.64	Joback Method
cpl	165.20	J/mol×K	298.15	NIST Webbook
cpl	166.52	J/mol×K	298.15	NIST Webbook
cpl	165.20	J/mol×K	298.15	NIST Webbook
cpl	166.24	J/mol×K	298.15	NIST Webbook
cpl	165.20	J/mol×K	298.15	NIST Webbook
cpl	161.10	J/mol×K	298.15	NIST Webbook
dvisc	0.0011710	Pa×s	298.15	Excess Molar Volumes and Deviations in Viscosity of Binary Mixtures of N,N-Dimethylformamide with Aniline and Benzonitrile at (298.15, 303.15, 308.15, and 313.15) K
dvisc	0.0010010	Pa×s	313.15	Excess Molar Volumes and Deviations in Viscosity of Binary Mixtures of N,N-Dimethylformamide with Aniline and Benzonitrile at (298.15, 303.15, 308.15, and 313.15) K
dvisc	0.0010680	Pa×s	308.15	Excess Molar Volumes and Deviations in Viscosity of Binary Mixtures of N,N-Dimethylformamide with Aniline and Benzonitrile at (298.15, 303.15, 308.15, and 313.15) K

dvisc	0.0011260	Pa×s	303.15	Excess Molar Volumes and Deviations in Viscosity of Binary Mixtures of N,N-Dimethylformamide with Aniline and Benzonitrile at (298.15, 303.15, 308.15, and 313.15) K
hfust	10.98	kJ/mol	260.30	NIST Webbook
hfust	10.98	kJ/mol	260.30	NIST Webbook
hfust	10.98	kJ/mol	260.33	NIST Webbook
hfust	10.98	kJ/mol	260.33	NIST Webbook
hfust	10.98	kJ/mol	260.33	NIST Webbook
hvapt	47.45	kJ/mol	464.10	KDB
hvapt	49.10	kJ/mol	382.50	NIST Webbook
rfi	1.53120		279.49	The measurements of coexistence curves and light scattering for {xC6H5CN + (1-x)CH3(CH2)6CH3} in the critical region
rfi	1.52990		281.97	The measurements of coexistence curves and light scattering for {xC6H5CN + (1-x)CH3(CH2)6CH3} in the critical region
rfi	1.53050		280.86	The measurements of coexistence curves and light scattering for {xC6H5CN + (1-x)CH3(CH2)6CH3} in the critical region
rfi	1.53070		280.38	The measurements of coexistence curves and light scattering for {xC6H5CN + (1-x)CH3(CH2)6CH3} in the critical region

rfi	1.53070		280.36	The measurements of coexistence curves and light scattering for {xC6H5CN + (1-x)CH3(CH2)6CH3} in the critical region
rfi	1.53210		277.43	The measurements of coexistence curves and light scattering for {xC6H5CN + (1-x)CH3(CH2)6CH3} in the critical region
rfi	1.53180		278.33	The measurements of coexistence curves and light scattering for {xC6H5CN + (1-x)CH3(CH2)6CH3} in the critical region
rfi	1.52890		284.13	The measurements of coexistence curves and light scattering for {xC6H5CN + (1-x)CH3(CH2)6CH3} in the critical region
rhol	982.50	kg/m3	318.15	Thermophysical and optical studies of molecular interactions in binary mixtures of diethyl carbonate with aromatic compounds at temperatures from 298.15 to 323.15 K
rhol	982.96	kg/m3	318.15	Measurements of Density and Heat Capacity for Binary Mixtures {x Benzonitrile + (1 -x) (Octane or Nonane)}
rhol	987.40	kg/m3	313.15	Measurements of Density and Heat Capacity for Binary Mixtures {x Benzonitrile + (1 -x) (Octane or Nonane)}

rhol	991.83	kg/m3	308.15	Measurements of Density and Heat Capacity for Binary Mixtures {x Benzonitrile + (1 -x) (Octane or Nonane)}
rhol	1005.12	kg/m3	293.15	Measurements of Density and Heat Capacity for Binary Mixtures {x Benzonitrile + (1 -x) (Octane or Nonane)}
rhol	1010.00	kg/m3	288.00	KDB
rhol	995.90	kg/m3	303.15	Thermophysical and optical studies of molecular interactions in binary mixtures of diethyl carbonate with aromatic compounds at temperatures from 298.15 to 323.15 K
rhol	991.40	kg/m3	308.15	Thermophysical and optical studies of molecular interactions in binary mixtures of diethyl carbonate with aromatic compounds at temperatures from 298.15 to 323.15 K
rhol	986.90	kg/m3	313.15	Thermophysical and optical studies of molecular interactions in binary mixtures of diethyl carbonate with aromatic compounds at temperatures from 298.15 to 323.15 K
rhol	996.26	kg/m3	303.15	Measurements of Density and Heat Capacity for Binary Mixtures {x Benzonitrile + (1 -x) (Octane or Nonane)}

rhol	1000.69	kg/m3	298.15	Measurements of Density and Heat Capacity for Binary Mixtures {x Benzonitrile + (1 -x) (Octane or Nonane)}
rhol	1009.55	kg/m3	288.15	Measurements of Density and Heat Capacity for Binary Mixtures {x Benzonitrile + (1 -x) (Octane or Nonane)}
rhol	1013.99	kg/m3	283.15	Measurements of Density and Heat Capacity for Binary Mixtures {x Benzonitrile + (1 -x) (Octane or Nonane)}
rhol	977.90	kg/m3	323.15	Thermophysical and optical studies of molecular interactions in binary mixtures of diethyl carbonate with aromatic compounds at temperatures from 298.15 to 323.15 K
rhol	1012.21	kg/m3	285.15	Measurements of Density and Heat Capacity for Binary Mixtures {x Benzonitrile + (1 -x) (Octane or Nonane)}
rhol	1000.60	kg/m3	298.15	Thermophysical and optical studies of molecular interactions in binary mixtures of diethyl carbonate with aromatic compounds at temperatures from 298.15 to 323.15 K
sfust	42.16	J/mol×K	260.33	NIST Webbook
sfust	42.16	J/mol×K	260.33	NIST Webbook
sfust	42.16	J/mol×K	260.33	NIST Webbook

speedsl	1368.20	m/s	313.15	Densities, speeds of sound and excess properties of (benzonitrile + methyl methacrylate, or + ethyl methacrylate, or + n-butyl methacrylate) binary mixtures at temperatures from 293.15 K to 318.15 K	
speedsl	1436.90	m/s	293.15	Densities, speeds of sound and excess properties of (benzonitrile + methyl methacrylate, or + ethyl methacrylate, or + n-butyl methacrylate) binary mixtures at temperatures from 293.15 K to 318.15 K	
speedsl	1352.90	m/s	318.15	Densities, speeds of sound and excess properties of (benzonitrile + methyl methacrylate, or + ethyl methacrylate, or + n-butyl methacrylate) binary mixtures at temperatures from 293.15 K to 318.15 K	
speedsl	1384.00	m/s	308.15	Densities, speeds of sound and excess properties of (benzonitrile + methyl methacrylate, or + ethyl methacrylate, or + n-butyl methacrylate) binary mixtures at temperatures from 293.15 K to 318.15 K	

speedsl	1400.70	m/s	303.15	Densities, speeds of sound and excess properties of (benzonitrile + methyl methacrylate, or + ethyl methacrylate, or + n-butyl methacrylate) binary mixtures at temperatures from 293.15 K to 318.15 K
speedsl	1418.20	m/s	298.15	Densities, speeds of sound and excess properties of (benzonitrile + methyl methacrylate, or + ethyl methacrylate, or + n-butyl methacrylate) binary mixtures at temperatures from 293.15 K to 318.15 K
srf	0.04	N/m	293.20	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	342.00	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49604e+01
Coeff. B	-4.30561e+03
Coeff. C	-4.76780e+01
Temperature range (K), min.	341.12
Temperature range (K), max.	493.91

Sources

Liquid-Liquid Equilibria for Water + Benzonitrile + N-Methylacetamide, or + N,N-Dimethylacetamide:	https://www.doi.org/10.1021/je9007074
Measurements of Density and Heat Capacity for Binary Mixtures {x Benzonitrile + (1- x) Octane or Decane}:	https://www.doi.org/10.1021/je100145f
Diffusion of Benzonitrile in CO2-Expanded Ethanol:	https://www.doi.org/10.1021/je800211x
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1396
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Excess Molar Volumes and Deviations in Viscosity of Binary Mixtures of N,N-Dimethylformamide with Aniline and Benzonitrile at (298.15, 303.15, 308.15, and 313.15) K:	https://www.doi.org/10.1021/je030101n
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100470&Units=SI
Liquid-Liquid Equilibria of Water + Benzonitrile + Propanone, or + Dimethyl Sulfoxide:	https://www.doi.org/10.1021/je030115t
Thermophysical and optical studies of molecular interactions in binary mixtures of diethyl carbonate with some benzene derivatives at temperatures from 298.15 to 323.15 K:	https://www.doi.org/10.1016/j.jct.2016.08.001
Densities, speeds of sound and excess properties of (benzonitrile + methyl or n-butyl methacrylate) binary mixtures at temperatures from 293.15 K to 318.15 K:	https://www.doi.org/10.1016/j.jct.2018.12.031
Thermodynamics of mixtures involving benzonitrile at temperatures from 293.15 to 323.15 K. Methacrylate, or n-butyl methacrylate) binary mixtures:	https://www.doi.org/10.1016/j.jct.2006.09.007
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Liquid-Liquid Equilibria for Water + Benzonitrile + Ethyl Acetate or + Butyl Acetate:	https://www.doi.org/10.1021/je050051h
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
The measurements of coexistence curves and light scattering for {xC6H5CN + (1- x)CH3(CH2)6CH3} in the critical region:	https://www.doi.org/10.1016/j.jct.2008.07.008

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
fpo:	Flash Point (Open Cup Method)
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
rhoc:	Critical density
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
speedsl:	Speed of sound in fluid
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume