

Butanenitrile

Other names:	1-CYANOPROPANE
	1-propanecarbonitrile
	BUTYRIC ACID NITRILE
	Butyronitrile
	Butyrylonitrile
	N-BUTYRONITRILE
	NSC 8412
	PROPYL CYANIDE
	Propylkyanid
	UN 2411
	butanonitrile
	n-Butanenitrile
	n-Butanitrile
	n-C3H7CN
	n-propyl cyanide
Inchi:	InChI=1S/C4H7N/c1-2-3-4-5/h2-3H2,1H3
InchiKey:	KVNRLNFWIYMESJ-UHFFFAOYSA-N
Formula:	C4H7N
SMILES:	CCCC#N
Mol. weight [g/mol]:	69.11
CAS:	109-74-0

Physical Properties

Property code	Value	Unit	Source
af	0.3730		KDB
affp	798.40	kJ/mol	NIST Webbook
basg	767.70	kJ/mol	NIST Webbook
chg	-2568.70 ± 0.92	kJ/mol	NIST Webbook
chl	-2579.00	kJ/mol	NIST Webbook
dm	3.80	debye	KDB
ea	0.02 ± 0.00	eV	NIST Webbook
gf	108.70	kJ/mol	KDB
hf	31.20	kJ/mol	NIST Webbook
hf	34.10	kJ/mol	KDB
hfl	-5.80 ± 1.00	kJ/mol	NIST Webbook
hfus	7.62	kJ/mol	Joback Method
hvap	34.98	kJ/mol	Joback Method

ie	11.67 ± 0.05	eV	NIST Webbook
ie	11.74	eV	NIST Webbook
ie	11.74	eV	NIST Webbook
ie	11.80 ± 0.25	eV	NIST Webbook
ie	11.20	eV	NIST Webbook
log10ws	-1.36		Crippen Method
logp	1.310		Crippen Method
mcvol	68.600	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=3)		KDB
pc	3880.00 ± 10.00	kPa	NIST Webbook
pc	3799.69 ± 81.06	kPa	NIST Webbook
pc	3789.55 ± 81.06	kPa	NIST Webbook
pc	3779.42 ± 81.06	kPa	NIST Webbook
pc	3779.42 ± 81.06	kPa	NIST Webbook
pc	3790.00 ± 91.19	kPa	NIST Webbook
pc	3880.00	kPa	KDB
rinpol	638.86		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	638.86		NIST Webbook
rinpol	643.90		NIST Webbook
rinpol	635.94		NIST Webbook
rinpol	636.93		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	619.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	639.74		NIST Webbook
rinpol	640.72		NIST Webbook
rinpol	641.67		NIST Webbook
rinpol	642.74		NIST Webbook
rinpol	643.90		NIST Webbook
rinpol	645.19		NIST Webbook
rinpol	646.43		NIST Webbook
rinpol	647.77		NIST Webbook
rinpol	649.23		NIST Webbook
rinpol	635.94		NIST Webbook

rinpol	635.87		NIST Webbook
rinpol	635.97		NIST Webbook
rinpol	636.14		NIST Webbook
rinpol	636.54		NIST Webbook
rinpol	636.93		NIST Webbook
rinpol	637.50		NIST Webbook
rinpol	638.14		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	638.10		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	622.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	619.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	633.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1100.00		NIST Webbook
tb	390.70	K	KDB
tb	390.55	K	Measurements of Quaternary Liquid-Liquid Equilibrium for Water + Acetic Acid + Propionic Acid + Solvent (Butyronitrile, Benzyl Acetate, or Methyl Isobutyl Ketone) at 298.15 K
tc	582.25 ± 0.90	K	NIST Webbook
tc	582.10 ± 2.00	K	NIST Webbook
tc	585.40 ± 0.20	K	NIST Webbook
tc	585.40	K	KDB
tc	582.15 ± 0.90	K	NIST Webbook
tf	161.25 ± 0.50	K	NIST Webbook
tf	160.90 ± 0.50	K	NIST Webbook
tf	160.00 ± 2.00	K	NIST Webbook
tf	161.15 ± 0.50	K	NIST Webbook
tf	161.25 ± 0.60	K	NIST Webbook
tf	161.20	K	KDB
vc	0.285	m3/kmol	KDB
zc	0.2275880		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.77	J/mol×K	553.11	Joback Method
cpg	136.66	J/mol×K	489.07	Joback Method
cpg	130.74	J/mol×K	457.04	Joback Method
cpg	124.57	J/mol×K	425.02	Joback Method
cpg	118.15	J/mol×K	393.00	Joback Method
cpg	152.98	J/mol×K	585.13	Joback Method
cpg	142.33	J/mol×K	521.09	Joback Method
cpl	134.20	J/mol×K	298.15	NIST Webbook
cpl	134.90	J/mol×K	303.15	NIST Webbook
dvisc	0.0005463	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	0.0005255	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
dvisc	0.0005049	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
hvapt	34.39	kJ/mol	390.40	KDB

hvapt	33.68	kJ/mol	390.80	NIST Webbook
hvapt	37.70	kJ/mol	366.50	NIST Webbook
hvapt	38.80	kJ/mol	398.00	NIST Webbook
rhoI	781.63	kg/m3	303.15	Density and Surface Tension of Binary Mixtures of 2,2,4-Trimethylpentane + n-Heptane, 2,2,4-Trimethylpentane + n-Octane, Ethyl Acetate + Benzene, and Butanenitrile + Benzene from (293.15 to 323.15) K
rhoI	786.27	kg/m3	298.15	Calorimetric Study of Nitrile Group-Solvent Interactions and Comparison with Dispersive Quasi-Chemical (DISQUAC) Predictions
rhoI	762.93	kg/m3	323.15	Density and Surface Tension of Binary Mixtures of 2,2,4-Trimethylpentane + n-Heptane, 2,2,4-Trimethylpentane + n-Octane, Ethyl Acetate + Benzene, and Butanenitrile + Benzene from (293.15 to 323.15) K
rhoI	767.64	kg/m3	318.15	Density and Surface Tension of Binary Mixtures of 2,2,4-Trimethylpentane + n-Heptane, 2,2,4-Trimethylpentane + n-Octane, Ethyl Acetate + Benzene, and Butanenitrile + Benzene from (293.15 to 323.15) K

rhoI	772.32	kg/m3	313.15	Density and Surface Tension of Binary Mixtures of 2,2,4-Trimethylpentane + n-Heptane, 2,2,4-Trimethylpentane + n-Octane, Ethyl Acetate + Benzene, and Butanenitrile + Benzene from (293.15 to 323.15) K
rhoI	776.99	kg/m3	308.15	Density and Surface Tension of Binary Mixtures of 2,2,4-Trimethylpentane + n-Heptane, 2,2,4-Trimethylpentane + n-Octane, Ethyl Acetate + Benzene, and Butanenitrile + Benzene from (293.15 to 323.15) K
rhoI	786.25	kg/m3	298.15	Density and Surface Tension of Binary Mixtures of 2,2,4-Trimethylpentane + n-Heptane, 2,2,4-Trimethylpentane + n-Octane, Ethyl Acetate + Benzene, and Butanenitrile + Benzene from (293.15 to 323.15) K
rhoI	790.86	kg/m3	293.15	Density and Surface Tension of Binary Mixtures of 2,2,4-Trimethylpentane + n-Heptane, 2,2,4-Trimethylpentane + n-Octane, Ethyl Acetate + Benzene, and Butanenitrile + Benzene from (293.15 to 323.15) K
rhoI	792.00	kg/m3	293.00	KDB
srf	0.03	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49287e+01
Coeff. B	-3.66225e+03
Coeff. C	-3.57970e+01
Temperature range (K), min.	285.93
Temperature range (K), max.	416.60

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	7.37325e+01
Coeff. B	-7.11602e+03
Coeff. C	-8.67200e+00
Coeff. D	5.60073e-06
Temperature range (K), min.	161.25
Temperature range (K), max.	582.25

Sources

KDB Vapor Pressure Data:

Molecular interaction studies and theoretical estimation of ultrasonic speed using the NRTL theory in Group-Solvent Interactions and Solubility with Dispersive Forces: Comparison with Different Quasi-Chemical (DISQUAC) Predictions

NIST Webbook:

Crippen Method:

Experimental (Solid + Liquid) and (Liquid + Liquid) Equilibria and Excess Volume of Alkanol + Acetonitrile, Propanenitrile, and Butanenitrile Mixtures:

Measurements of Quaternary Liquid-Liquid Equilibrium for Water + Acetic Acid + Propionic Acid + Solvent (Butyronitrile, Benzyl Acetate, or Methyl isobutyl Ketone) at 298.15 K:

Densities and Surface Tension of Binary Mixtures of 2,2,4-Trimethylpentane + n-Heptane, 2,2,4-Trimethylpentane + n-Octane, Ethyl Acetate + Benzene, and Butanenitrile + Benzene from (293.15 to 323.15) K:

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1388>

<https://www.doi.org/10.1016/j.tca.2009.10.001>

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

<https://www.doi.org/10.1021/je050262m>

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

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<https://www.doi.org/10.1021/je050527x>

<http://pubs.acs.org/doi/abs/10.1021/ci990307i>

<https://www.doi.org/10.1021/acs.jced.5b00009>

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
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
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
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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