Pentanenitrile

Other names:	1-Butyl cyanide
	1-CYANOBUTANE
	BUTYL CYANIDE
	Butane, 1-cyano-
	CH3(CH2)3CN
	N-VALERONITRILE
	Pentanonitrile
	VALERONITRILE
	n-Pentanenitrile
Inchi:	InChI=1S/C5H9N/c1-2-3-4-5-6/h2-4H2,1H3
InchiKey:	RFFFKMOABOFIDF-UHFFFAOYSA-N
Formula:	C5H9N
SMILES:	CCCCC#N
Mol. weight [g/mol]:	83.13
CAS:	110-59-8

Physical Properties

Property code	Value	Unit	Source
affp	802.40	kJ/mol	NIST Webbook
basg	771.70	kJ/mol	NIST Webbook
chl	-3220.70 ± 1.30	kJ/mol	NIST Webbook
ea	0.01 ± 0.00	eV	NIST Webbook
gf	124.40	kJ/mol	Joback Method
hf	11.10	kJ/mol	NIST Webbook
hfl	-33.20	kJ/mol	NIST Webbook
hfus	10.21	kJ/mol	Joback Method
hvap	44.27	kJ/mol	NIST Webbook
hvap	44.10 ± 0.20	kJ/mol	NIST Webbook
hvap	44.30	kJ/mol	NIST Webbook
hvap	44.30	kJ/mol	NIST Webbook
hvap	43.60 ± 0.10	kJ/mol	NIST Webbook
hvap	43.64	kJ/mol	NIST Webbook
log10ws	-1.78		Crippen Method
logp	1.700		Crippen Method
mcvol	82.690	ml/mol	McGowan Method
pc	3580.00 ± 10.00	kPa	NIST Webbook
pc	3580.00	kPa	KDB

rinpol	754.80	NIST Webbook
rinpol	737.27	NIST Webbook
rinpol	737.44	NIST Webbook
rinpol	753.12	NIST Webbook
rinpol	738.24	NIST Webbook
rinpol	738.84	NIST Webbook
rinpol	739.50	NIST Webbook
rinpol	740.32	NIST Webbook
rinpol	741.21	NIST Webbook
rinpol	778.42	NIST Webbook
rinpol	692.90	NIST Webbook
rinpol	693.60	NIST Webbook
rinpol	751.52	NIST Webbook
rinpol	755.00	NIST Webbook
rinpol	736.00	NIST Webbook
rinpol	738.00	NIST Webbook
rinpol	738.00	NIST Webbook
rinpol	749.97	NIST Webbook
rinpol	721.00	NIST Webbook
rinpol	772.90	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	741.00	NIST Webbook
rinpol	742.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	744.00	NIST Webbook
rinpol	747.00	NIST Webbook
rinpol	741.00	NIST Webbook
rinpol	736.00	NIST Webbook
rinpol	721.00	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	721.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	747.00	NIST Webbook
rinpol	772.90	NIST Webbook
rinpol	748.48	NIST Webbook
rinpol	747.03	NIST Webbook
rinpol	745.75	NIST Webbook
rinpol	744.50	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	743.33	NIST Webbook
rinpol	742.19	NIST Webbook
rinpol	745.00	NIST Webbook
rinpol	737.79	NIST Webbook

tb	413.90 ± 0.30	K	NIST Webbook
tb	391.70 ± 20.00	K	NIST Webbook
tb	413.00 ± 2.00	K	NIST Webbook
tb	414.00 ± 2.00	K	NIST Webbook
tb	413.00 ± 4.00	K	NIST Webbook
tb	413.90 ± 0.30	K	NIST Webbook
tb	414.40	K	KDB
tb	413.20	K	NIST Webbook
tb	413.00 ± 1.00	K	NIST Webbook
tb	414.50	K	NIST Webbook
tb	414.40	K	NIST Webbook
tb	413.60 ± 0.50	K	NIST Webbook
tb	415.00 ± 2.00	K	NIST Webbook
tb	414.40 ± 1.00	K	NIST Webbook
tb	413.00 ± 5.00	K	NIST Webbook
tb	414.40 ± 0.07	K	NIST Webbook
tb	414.50 ± 0.70	K	NIST Webbook
tb	409.00 ± 5.00	K	NIST Webbook
tb	414.00 ± 2.00	K	NIST Webbook
tb	419.85 ± 0.20	K	NIST Webbook
tb	414.50 ± 0.30	K	NIST Webbook
tb	413.30 ± 1.00	K	NIST Webbook
tc	610.30	K	KDB
tc	610.30 ± 0.20	K	NIST Webbook
tf	176.95 ± 0.15	K	NIST Webbook
tf	176.37 ± 0.05	K	NIST Webbook
tf	177.00 ± 2.00	K	NIST Webbook
tf	177.00 ± 2.00	K	NIST Webbook
tf	176.90	K	KDB
tf	176.92 ± 0.20	K	NIST Webbook
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.68	J/mol×K	606.51	Joback Method
cpg	160.74	J/mol×K	447.65	Joback Method
cpg	152.81	J/mol×K	415.88	Joback Method
cpg	189.29	J/mol×K	574.74	Joback Method
cpg	182.62	J/mol×K	542.97	Joback Method
cpg	175.64	J/mol×K	511.20	Joback Method

cpg	168.35	J/mol×K	479.42	Joback Method
hvapt	42.30	kJ/mol	365.50	NIST Webbook
hvapt	44.20	kJ/mol	378.00	NIST Webbook
hvapt	36.09	kJ/mol	414.40	NIST Webbook
pvap	20.00	kPa	362.77	Physico-Chemical Properties of LiFSI Solutions I. LiFSI with Valeronitrile, Dichloromethane, 1,2-Dichloroethane, and 1,2-Dichlorobenzene
pvap	9.90	kPa	344.89	Physico-Chemical Properties of LiFSI Solutions I. LiFSI with Valeronitrile, Dichloromethane, 1,2-Dichloroethane, and 1,2-Dichlorobenzene
pvap	5.00	kPa	329.35	Physico-Chemical Properties of LiFSI Solutions I. LiFSI with Valeronitrile, Dichloromethane, 1,2-Dichloroethane, and 1,2-Dichlorobenzene
pvap	100.00	kPa	412.96	Physico-Chemical Properties of LiFSI Solutions I. LiFSI with Valeronitrile, Dichloromethane, 1,2-Dichloroethane, and 1,2-Dichlorobenzene
pvap	30.00	kPa	374.08	Physico-Chemical Properties of LiFSI Solutions I. LiFSI with Valeronitrile, Dichloromethane, 1,2-Dichloroethane, and 1,2-Dichlorobenzene

pvap	45.00	kPa	386.22	Physico-Chemical Properties of LiFSI Solutions I. LiFSI with Valeronitrile, Dichloromethane, 1,2-Dichloroethane, and 1,2-Dichlorobenzene
pvap	60.00	kPa	395.40	Physico-Chemical Properties of LiFSI Solutions I. LiFSI with Valeronitrile, Dichloromethane, 1,2-Dichloroethane, and 1,2-Dichlorobenzene
pvap	86.40	kPa	407.76	Physico-Chemical Properties of LiFSI Solutions I. LiFSI with Valeronitrile, Dichloromethane, 1,2-Dichloroethane, and 1,2-Dichlorobenzene
pvap	95.00	kPa	411.12	Physico-Chemical Properties of LiFSI Solutions I. LiFSI with Valeronitrile, Dichloromethane, 1,2-Dichloroethane, and 1,2-Dichlorobenzene
pvap	10.00	kPa	345.13	Physico-Chemical Properties of LiFSI Solutions I. LiFSI with Valeronitrile, Dichloromethane, 1,2-Dichloroethane, and 1,2-Dichlorobenzene
rhol	794.79	kg/m3	298.15	Calorimetric Study of Nitrile Group-Solvent Interactions and Comparison with Dispersive Quasi-Chemical (DISQUAC) Predictions

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49756e+01
Coeff. B	-3.84562e+03
Coeff. C	-4.27040e+01
Temperature range (K), min.	304.52
Temperature range (K), max.	440.63

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.00058e+02
Coeff. B	-8.56597e+03
Coeff. C	-1.26679e+01
Coeff. D	9.19771e-06
Temperature range (K), min.	176.95
Temperature range (K), max.	603.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Calorimetric Study of Nitrile Group-Solvent Interactions and Comparison with Dispersive Quasi-Chemical (DISQUAC) Predictions:	https://www.doi.org/10.1021/je100489z
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1390
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1390
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110598&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
High pressure phase behavior for the binary mixture of valeronitrile, capronitrile and n-butane in supercritical carbon dioxide at temperatures from 313.2 to 393.2 K and pressures from 8.9 to 25.7 MPa:	https://www.doi.org/10.1016/j.fluid.2011.09.019
Physico-Chemical Properties of LiFSI Solutions. LiFSI with Valeronitrile, Crippen Method - 1,2-Dichloroethane and 1,2-Dichlorobenzene:	https://www.doi.org/10.1021/acs.jced.8b00590 https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume