3-Pentenenitrile

Other names:	1-cyano-2-butene
	2-cyano-2-butene
	2-methyl-2-butenenitrile
	3-Pentenonitrile
	crotyl cyanide
	pent-3-enenitrile
Inchi:	InChI=1S/C5H7N/c1-2-3-4-5-6/h2-3H,4H2,1H3
InchiKey:	UVKXJAUUKPDDNW-UHFFFAOYSA-N
Formula:	C5H7N
SMILES:	CC=CCC#N
Mol. weight [g/mol]:	81.12
CAS:	4635-87-4

Physical Properties

Property code	Value	Unit	Source
gf	204.62	kJ/mol	Joback Method
hf	135.57	kJ/mol	Joback Method
hfus	10.41	kJ/mol	Joback Method
hvap	37.16	kJ/mol	Joback Method
log10ws	-0.96		Aqueous Solubility Prediction Method
logp	1.476		Crippen Method
mcvol	78.390	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
tb	418.50 ± 1.50	K	NIST Webbook
tc	620.58	K	Joback Method
tf	206.02	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.82	J/mol×K	420.04	Joback Method
cpg	144.23	J/mol×K	453.46	Joback Method

cpg	151.25	J/mol×K	486.89	Joback Method
cpg	157.88	J/mol×K	520.31	Joback Method
cpg	164.16	J/mol×K	553.73	Joback Method
cpg	170.09	J/mol×K	587.15	Joback Method
cpg	175.70	J/mol×K	620.58	Joback Method
pvap	35.37	kPa	382.01	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa
pvap	9.49	kPa	344.85	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa
pvap	13.48	kPa	353.91	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa
pvap	18.32	kPa	362.45	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa

pvap	22.91	kPa	368.92	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa
pvap	28.80	kPa	375.61	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa
pvap	7.59	kPa	339.24	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa
pvap	40.09	kPa	386.13	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa
pvap	42.83	kPa	388.17	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa

pvap	47.08	kPa	391.42	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa
pvap	51.62	kPa	394.31	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa
pvap	57.83	kPa	398.64	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa
pvap	65.49	kPa	402.51	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa
pvap	74.49	kPa	407.31	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa

pvap	80.01	kPa	409.72	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa
pvap	86.78	kPa	412.88	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa
pvap	90.50	kPa	414.32	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa
pvap	97.90	kPa	417.51	Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa
pvap	50.00	kPa	367.43	Isobaric Vapor Liquid Equilibria for Binary Mixtures of Z,E-2-Methyl-2-butenenitrile, R,S-4-Vinyl-1-cyclohexene, and Z,E-3-Pentenenitrile
pvap	100.00	kPa	392.75	Isobaric Vapor Liquid Equilibria for Binary Mixtures of Z,E-2-Methyl-2-butenenitrile, R,S-4-Vinyl-1-cyclohexene, and Z,E-3-Pentenenitrile

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46705e+01
Coeff. B	-3.62892e+03
Coeff. C	-5.74930e+01
Temperature range (K), min.	309.80
Temperature range (K), max.	445.24

Sources

Isobaric Vapor Liquid Equilibria for Binary Mixtures of Z,E-2-Methyl-2-butenenitrile, R,S-4-Vinyl-1-cyclohexene, and Z,E-3-Pentenenitrile:	https://www.doi.org/10.1021/acs.jced.6b00388
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4635874&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Vapor-Liquid Equilibrium for Binary Mixtures of 3-Cyano-1-butene + R,S-4-Vinyl-1-cyclohexene, 3-Cyano-1-butene + Z,E-1-Cyano-2-butene and R,S-4-Vinyl-1-cyclohexene + Z,E-3-pentenenitrile) at (50.0 and 100.0) kPa:	https://www.doi.org/10.1021/acs.jced.8b00158
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary systems (4-vinyl-1-cyclohexene + 2E-1-Cyano-2-butene:	https://www.doi.org/10.1016/j.jct.2015.08.015
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume