Octanenitrile

Other names:	1-Cyanoheptane
	Arneel 8
	Caprylnitrile
	Caprylonitrile
	Normal-heptyl cyanide
	Octanonitrile
	heptyl cyanide
	n-Heptyl cyanide
Inchi:	InChI=1S/C8H15N/c1-2-3-4-5-6-7-8-9/h2-7H2,1H3
InchiKey:	YSIMAPNUZAVQER-UHFFFAOYSA-N
Formula:	C8H15N
SMILES:	CCCCCCCC#N
Mol. weight [g/mol]:	125.21
CAS:	124-12-9

Physical Properties

Property code	Value	Unit	Source
affp	811.00	kJ/mol	NIST Webbook
affp	806.20	kJ/mol	NIST Webbook
chl	-5184.50 ± 1.00	kJ/mol	NIST Webbook
gf	149.66	kJ/mol	Joback Method
hf	-50.60 ± 1.50	kJ/mol	NIST Webbook
hfl	-107.40 ± 1.50	kJ/mol	NIST Webbook
hfus	17.98	kJ/mol	Joback Method
hvap	43.88	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.870		Crippen Method
mcvol	124.960	ml/mol	McGowan Method
pc	2850.00 ± 10.00	kPa	NIST Webbook
rinpol	1080.60		NIST Webbook
rinpol	1079.30		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	178.33		NIST Webbook
rinpol	1085.00		NIST Webbook
ripol	1512.00		NIST Webbook
ripol	1512.00		NIST Webbook

ripol	1462.00		NIST Webbook
tb	472.20	K	NIST Webbook
tb	478.40 ± 0.50	K	NIST Webbook
tb	473.00 ± 3.00	K	NIST Webbook
tb	478.40	K	NIST Webbook
tc	674.40 ± 0.20	K	NIST Webbook
tf	219.65 ± 0.50	K	NIST Webbook
tf	314.00 ± 2.00	K	NIST Webbook
tf	227.55 ± 1.00	K	NIST Webbook
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.20	J/mol×K	669.65	Joback Method
cpg	293.39	J/mol×K	546.23	Joback Method
cpg	282.27	J/mol×K	515.38	Joback Method
cpg	270.65	J/mol×K	484.52	Joback Method
cpg	323.92	J/mol×K	638.80	Joback Method
cpg	314.20	J/mol×K	607.94	Joback Method
cpg	304.03	J/mol×K	577.09	Joback Method
hvapt	49.80	kJ/mol	397.00	NIST Webbook
hvapt	48.00	kJ/mol	449.50	NIST Webbook
hvapt	56.70	kJ/mol	396.50	NIST Webbook
hvapt	50.00	kJ/mol	426.50	NIST Webbook
pvap	0.05	kPa	301.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.06	kPa	304.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.08	kPa	307.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

pvap	0.09	kPa	310.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.09	kPa	310.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.20e-04	kPa	238.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	2.10e-04	kPa	243.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	3.70e-04	kPa	248.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	0.05	kPa	301.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.08e-03	kPa	258.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	1.80e-03	kPa	263.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach

pvap	2.95e-03	kPa	268.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	4.76e-03	kPa	273.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	5.02e-03	kPa	273.65	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	7.58e-03	kPa	278.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	0.01	kPa	283.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	0.02	kPa	288.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	0.03	kPa	293.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach

pvap	0.04	kPa	298.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach	
pvap	0.06	kPa	303.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach	
pvap	0.08	kPa	308.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach	
pvap	0.04	kPa	298.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.	
pvap	0.03	kPa	295.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.	
pvap	0.02	kPa	292.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.	
pvap	0.02	kPa	289.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.	
pvap	0.02	kPa	286.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.	
pvap	0.01	kPa	283.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.	

pvap	6.40e-04	kPa	253.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51465e+01
Coeff. B	-4.19093e+03
Coeff. C	-7.41310e+01
Temperature range (K), min.	356.18
Temperature range (K), max.	500.25

Sources

Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach	https://www.doi.org/10.1021/acs.jced.8b00699
Excess Enthalpies of (CH3(CH2)nCN, n-5 to 12) + Methyl Methylthiomethyl Sulfoxide or + Dimethyl Sulfoxide at 298.15 K	https://www.doi.org/10.1021/je0499317
Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.:	https://www.doi.org/10.1016/j.jct.2004.08.004
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C124129&Units=SI

Legend

affp:	Proton affinity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume