Heptanonitrile

Other names:	1-Cyanohexane
	1-Heptanonitrile
	Enanthonitrile
	Heptanenitrile
	Heptyl nitrile
	Hexyl cyanide
	heptane-1-nitrile
	n-Heptanenitrile
	n-Hexyl cyanide
Inchi:	InChI=1S/C7H13N/c1-2-3-4-5-6-7-8/h2-6H2,1H3
InchiKey:	SDAXRHHPNYTELL-UHFFFAOYSA-N
Formula:	C7H13N
SMILES:	CCCCCCC#N
Mol. weight [g/mol]:	111.18
CAS:	629-08-3

Physical Properties

Property code	Value	Unit	Source
affp	809.00	kJ/mol	NIST Webbook
affp	805.40	kJ/mol	NIST Webbook
gf	141.24	kJ/mol	Joback Method
hf	-31.00 ± 1.00	kJ/mol	NIST Webbook
hfl	-82.80 ± 0.80	kJ/mol	NIST Webbook
hfus	15.39	kJ/mol	Joback Method
hvap	41.65	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.480		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	945.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	985.00		NIST Webbook
ripol	1405.00		NIST Webbook
ripol	1354.00		NIST Webbook
ripol	1396.00		NIST Webbook

ripol	1405.00		NIST Webbook
ripol	1396.00		NIST Webbook
tb	461.64	K	Joback Method
tc	648.70	K	Joback Method
tf	209.35 ± 0.50	K	NIST Webbook
tf	210.55 ± 2.00	K	NIST Webbook
tf	209.15 ± 0.50	K	NIST Webbook
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.78	J/mol×K	523.99	Joback Method
cpg	239.70	J/mol×K	492.82	Joback Method
cpg	285.87	J/mol×K	648.70	Joback Method
cpg	277.45	J/mol×K	617.53	Joback Method
cpg	268.64	J/mol×K	586.35	Joback Method
cpg	259.42	J/mol×K	555.17	Joback Method
cpg	229.18	J/mol×K	461.64	Joback Method
hvapt	46.40	kJ/mol	375.50	NIST Webbook
hvapt	46.00	kJ/mol	393.00	NIST Webbook
pvap	0.02	kPa	273.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	4.80e-04	kPa	238.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	8.50e-04	kPa	243.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach

pvap	1.46e-03	kPa	248.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	2.46e-03	kPa	253.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	4.08e-03	kPa	258.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	6.62e-03	kPa	263.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	0.01	kPa	268.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	0.21	kPa	307.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	273.66	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach

pvap	0.03	kPa	278.16	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	0.04	kPa	283.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	0.06	kPa	288.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	0.08	kPa	293.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	0.12	kPa	298.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	0.16	kPa	303.16	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	0.23	kPa	308.18	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach

pvap	0.17	kPa	304.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.14	kPa	301.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.11	kPa	298.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.09	kPa	295.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.08	kPa	292.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.06	kPa	289.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.05	kPa	286.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.04	kPa	283.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.03	kPa	280.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49789e+01
Coeff. B	-3.98492e+03
Coeff. C	-6.83770e+01
Temperature range (K), min.	339.62
Temperature range (K), max.	480.58

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
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629083&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

Legend

affp:	Proton affinity
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