

Nonanenitrile

Other names:	1-cyanooctane 1-octyl cyanide NSC 5560 Nonanetrile Nonanenitrile Nonanonitrile Nonyl nitrile Pelargononitrile n-Nonanenitrile n-Octylcyanide n-nonanonitrile n-octanenitrile n-octyl cyanide octyl cyanide pelargonitrile
Inchi:	InChI=1S/C9H17N/c1-2-3-4-5-6-7-8-9-10/h2-8H2,1H3
InchiKey:	PLZZPPHAMDJOSR-UHFFFAOYSA-N
Formula:	C9H17N
SMILES:	CCCCCCCCC#N
Mol. weight [g/mol]:	139.24
CAS:	2243-27-8

Physical Properties

Property code	Value	Unit	Source
affp	812.00	kJ/mol	NIST Webbook
affp	807.10	kJ/mol	NIST Webbook
gf	158.08	kJ/mol	Joback Method
hf	-64.21	kJ/mol	Joback Method
hfus	20.57	kJ/mol	Joback Method
hvap	62.00 ± 0.30	kJ/mol	NIST Webbook
hvap	58.00	kJ/mol	NIST Webbook
log10ws	-3.46		Crippen Method
logp	3.261		Crippen Method
mcvol	139.050	ml/mol	McGowan Method
pc	2252.53	kPa	Joback Method
rinpol	1185.00		NIST Webbook
rinpol	1182.20		NIST Webbook

rinpol	1182.20			NIST Webbook
rinpol	1185.00			NIST Webbook
rinpol	199.75			NIST Webbook
ripol	1593.00			NIST Webbook
ripol	1593.00			NIST Webbook
ripol	1565.00			NIST Webbook
ripol	1565.00			NIST Webbook
ripol	1593.00			NIST Webbook
tb	488.00 ± 8.00		K	NIST Webbook
tb	488.00 ± 5.00		K	NIST Webbook
tb	497.00 ± 1.00		K	NIST Webbook
tb	497.60		K	NIST Webbook
tc	690.60		K	Joback Method
tf	238.95 ± 1.00		K	NIST Webbook
tf	223.65 ± 0.50		K	NIST Webbook
vc	0.566		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.15	J/mol×K	507.40	Joback Method
cpg	326.75	J/mol×K	537.93	Joback Method
cpg	338.81	J/mol×K	568.47	Joback Method
cpg	350.34	J/mol×K	599.00	Joback Method
cpg	361.36	J/mol×K	629.53	Joback Method
cpg	371.88	J/mol×K	660.07	Joback Method
cpg	381.92	J/mol×K	690.60	Joback Method
hvapt	56.80	kJ/mol	415.50	NIST Webbook
pvap	0.02	kPa	304.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	4.49e-03	kPa	286.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	5.19e-03	kPa	288.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

pvap	6.40e-03	kPa	290.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	7.14e-03	kPa	291.70	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	7.97e-03	kPa	293.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	9.92e-03	kPa	295.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	296.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	298.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	299.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	301.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	302.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	3.90e-03	kPa	285.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

pvap	0.02	kPa	305.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	307.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.03	kPa	308.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.03	kPa	310.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.04	kPa	311.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.04	kPa	313.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.05	kPa	316.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.05	kPa	316.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.06	kPa	319.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.07	kPa	320.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

pvap	0.08	kPa	323.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.48e-03	kPa	273.66	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	2.31e-03	kPa	278.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	3.70e-03	kPa	283.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	5.85e-03	kPa	288.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	9.07e-03	kPa	293.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	0.01	kPa	298.15	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach

pvap	0.02	kPa	303.16	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach
pvap	0.03	kPa	308.18	Extracting Vapor Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach

Sources

Excess Enthalpies of {CH ₃ (CH ₂) _n CN, n = 5 to 12} + Methyl Methylthiomethyl Sulfide and Dimethyl Sulfoxide at 298.15 K: McGowan Method:	https://www.doi.org/10.1021/je0499317
NIST Webbook:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2243278&Units=SI
Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Alkylamines. Pressure Data from Gas-Liquid Chromatography Retention Times. Part 2: Analysis of Double Reference Approach:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
	https://www.chemeo.com/doc/models/crippen_log10ws
	https://www.doi.org/10.1016/j.jct.2004.08.004
	https://www.doi.org/10.1021/acs.jced.8b00699

Legend

affp:	Proton affinity
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
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

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