Decanenitrile

Other names:	1-Cyanononane
	1-Decanenitrile
	Caprinitrile
	Decanonitrile
	N-CAPRINITRILE
	NSC 6085
	Nitrile 10 D
	Nonyl cyanide
	n-Decanenitrile
	n-Nonyl cyanide
Inchi:	InChI=1S/C10H19N/c1-2-3-4-5-6-7-8-9-10-11/h2-9H2,1H3
InchiKey:	HBZDPWBWBJMYRY-UHFFFAOYSA-N
Formula:	C10H19N
SMILES:	CCCCCCCCCC#N
Mol. weight [g/mol]:	153.26
CAS:	1975-78-6

Physical Properties

Property code	Value	Unit	Source
chl	-6492.10 ± 1.20	kJ/mol	NIST Webbook
gf	166.50	kJ/mol	Joback Method
hf	-91.60 ± 1.80	kJ/mol	NIST Webbook
hfl	-158.40 ± 1.80	kJ/mol	NIST Webbook
hfus	23.16	kJ/mol	Joback Method
hvap	66.80	kJ/mol	NIST Webbook
hvap	66.80 ± 0.40	kJ/mol	NIST Webbook
hvap	66.84	kJ/mol	NIST Webbook
hvap	66.30 ± 0.40	kJ/mol	NIST Webbook
hvap	66.84 ± 0.37	kJ/mol	NIST Webbook
log10ws	-3.88		Crippen Method
logp	3.651		Crippen Method
mcvol	153.140	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	1286.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	219.15		NIST Webbook
rinpol	219.15		NIST Webbook

rinpol	1276.00		NIST Webbook
rinpol	1286.00		NIST Webbook
ripol	1677.00		NIST Webbook
tb	516.90 ± 1.50	K	NIST Webbook
tc	711.60	K	Joback Method
tf	255.25 ± 2.00	K	NIST Webbook
tf	258.69 ± 0.30	K	NIST Webbook
tf	258.69 ± 0.30	K	NIST Webbook
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.59	J/mol×K	530.28	Joback Method
cpg	373.05	J/mol×K	560.50	Joback Method
cpg	385.94	J/mol×K	590.72	Joback Method
cpg	398.26	J/mol×K	620.94	Joback Method
cpg	410.03	J/mol×K	651.16	Joback Method
cpg	421.27	J/mol×K	681.38	Joback Method
cpg	431.99	J/mol×K	711.60	Joback Method
hvapt	58.00	kJ/mol	450.00	NIST Webbook
hvapt	57.80	kJ/mol	406.00	NIST Webbook
hvapt	54.40	kJ/mol	474.50	NIST Webbook
pvap	4.84e-03	kPa	298.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	3.59e-03	kPa	295.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	6.92e-03	kPa	302.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	9.28e-03	kPa	305.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

pvap	0.01	kPa	308.70	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	311.70	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	313.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	315.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	316.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.03	kPa	319.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.03	kPa	322.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.05	kPa	326.30	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	1.46347e+01

Coeff. B	-4.32966e+03
Coeff. C	-8.46400e+01
Temperature range (K), min.	386.42
Temperature range (K), max.	549.04

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.47381e+02
Coeff. B	-1.32453e+04
Coeff. C	-1.91825e+01
Coeff. D	1.02455e-05
Temperature range (K), min.	342.15
Temperature range (K), max.	518.15

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1975786&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1394
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
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
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

Legend

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