

Undecanenitrile

Other names:	1-Cyanodecane 1-decylocyanide Undecanoic acid nitrile Undecanonitrile n-Decyl cyanide
Inchi:	InChI=1S/C11H21N/c1-2-3-4-5-6-7-8-9-10-11-12/h2-10H2,1H3
InchiKey:	SZKKNEOUHLFYNA-UHFFFAOYSA-N
Formula:	C11H21N
SMILES:	CCCCCCCCC#N
Mol. weight [g/mol]:	167.29
CAS:	2244-07-7

Physical Properties

Property code	Value	Unit	Source
chl	-7145.30 ± 1.30	kJ/mol	NIST Webbook
gf	174.92	kJ/mol	Joback Method
hf	-113.40 ± 2.00	kJ/mol	NIST Webbook
hfl	-184.50 ± 2.00	kJ/mol	NIST Webbook
hfus	25.75	kJ/mol	Joback Method
hvac	71.10 ± 0.10	kJ/mol	NIST Webbook
hvac	71.10	kJ/mol	NIST Webbook
hvac	71.14 ± 0.14	kJ/mol	NIST Webbook
hvac	71.80 ± 0.30	kJ/mol	NIST Webbook
hvac	71.14	kJ/mol	NIST Webbook
log10ws	-4.29		Crippen Method
logp	4.041		Crippen Method
mccol	167.230	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	237.44		NIST Webbook
tb	526.20	K	NIST Webbook
tc	732.71	K	Joback Method
tf	267.35 ± 1.00	K	NIST Webbook
vc	0.677	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.09	J/mol×K	583.08	Joback Method
cpg	483.36	J/mol×K	732.71	Joback Method
cpg	472.04	J/mol×K	702.78	Joback Method
cpg	460.16	J/mol×K	672.86	Joback Method
cpg	447.72	J/mol×K	642.93	Joback Method
cpg	434.71	J/mol×K	613.01	Joback Method
cpg	406.85	J/mol×K	553.16	Joback Method
hvapt	63.70	kJ/mol	444.50	NIST Webbook
pvap	0.02	kPa	328.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	8.77e-03	kPa	319.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	322.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	322.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	325.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	325.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	327.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

pvap	8.34e-03	kPa	319.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	331.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	332.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.03	kPa	334.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.03	kPa	337.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.04	kPa	337.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.04	kPa	340.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	5.77e-03	kPa	314.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	5.10e-03	kPa	313.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	4.02e-03	kPa	310.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

pvap	3.74e-03	kPa	309.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	3.08e-03	kPa	307.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	2.55e-03	kPa	305.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.31e-03	kPa	298.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	6.20e-04	kPa	290.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52806e+01
Coeff. B	-4.65763e+03
Coeff. C	-8.93660e+01
Temperature range (K), min.	400.02
Temperature range (K), max.	556.57

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2244077&Units=SI>

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/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles of (CH₃(CH₂)_nCN, n = 5 to 12) + Methyl Methylthiomethyl Sulfide and Dimethyl Sulfoxide at 298.15 K: <https://www.doi.org/10.1016/j.jct.2004.08.004>
McGowan Method: <https://www.doi.org/10.1021/je0499317>
https://en.wikipedia.org/wiki/Joback_method
<http://link.springer.com/article/10.1007/BF02311772>

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

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