

Dodecanenitrile

Other names:	1-Cyanoundecane Decylacetonitrile Dodecanonitrile Lauric acid nitrile Lauric nitrile Lauronitrile NSC 1804 Nitrile 12 Undecyl cyanide n-Undecyl cyanide n-dodecanenitrile
Inchi:	InChI=1S/C12H23N/c1-2-3-4-5-6-7-8-9-10-11-12-13/h2-11H2,1H3
InchiKey:	VXCUURYWGLIH-UHFFFAOYSA-N
Formula:	C12H23N
SMILES:	CCCCCCCCCCC#N
Mol. weight [g/mol]:	181.32
CAS:	2437-25-4

Physical Properties

Property code	Value	Unit	Source
gf	183.34	kJ/mol	Joback Method
hf	-126.13	kJ/mol	Joback Method
hfus	28.34	kJ/mol	Joback Method
hvap	74.90 ± 0.20	kJ/mol	NIST Webbook
hvap	76.12	kJ/mol	NIST Webbook
hvap	76.10 ± 0.10	kJ/mol	NIST Webbook
log10ws	-4.71		Crippen Method
logp	4.431		Crippen Method
mvol	181.320	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	1490.00		NIST Webbook
rinpol	254.48		NIST Webbook
rinpol	254.48		NIST Webbook
tb	550.20	K	NIST Webbook
tc	753.98	K	Joback Method
tf	277.15 ± 1.00	K	NIST Webbook
tf	277.17 ± 0.30	K	NIST Webbook

tf	277.17 ± 0.30	K	NIST Webbook
tf	277.05 ± 0.30	K	NIST Webbook
tf	276.65 ± 2.00	K	NIST Webbook
vc	0.734	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.02	J/mol×K	635.35	Joback Method
cpg	470.75	J/mol×K	605.70	Joback Method
cpg	535.99	J/mol×K	753.98	Joback Method
cpg	524.13	J/mol×K	724.32	Joback Method
cpg	511.69	J/mol×K	694.67	Joback Method
cpg	498.66	J/mol×K	665.01	Joback Method
cpg	455.83	J/mol×K	576.04	Joback Method
hvapt	65.20	kJ/mol	427.50	NIST Webbook
hvapt	60.70	kJ/mol	498.00	NIST Webbook
pvap	0.03	kPa	349.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	9.36e-03	kPa	331.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	334.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	337.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	340.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

pvap	0.02	kPa	343.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.03	kPa	346.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	7.42e-03	kPa	328.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.04	kPa	352.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.05	kPa	355.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.06	kPa	358.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.08	kPa	361.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.09	kPa	364.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.11	kPa	367.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	5.90e-03	kPa	325.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

pvap	4.62e-03	kPa	322.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	3.60e-03	kPa	319.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	3.23e-03	kPa	318.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	2.39e-03	kPa	315.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.86e-03	kPa	312.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.11e-03	kPa	306.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	7.10e-04	kPa	301.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	5.20e-04	kPa	298.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	471.20	K	13.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47501e+01
Coeff. B	-4.62117e+03
Coeff. C	-9.40920e+01
Temperature range (K), min.	413.62
Temperature range (K), max.	583.70

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
High pressure phase behavior for the binary mixture of valeronitrile, Vapor Pressure and Enthalpies of Vaporization and Entropy of Vaporization of a Series of the Linear Alkanes from 313.2 to 393.2 K and pressures from 3.9 to 25.7 MPa:	https://www.doi.org/10.1016/j.fluid.2011.09.019
Crippen Method:	https://www.doi.org/10.1016/j.jct.2004.08.004
Joback Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2437254&Units=SI
Excess Enthalpies of {CH ₃ (CH ₂) _n CN, n = 5 to 12} + Methyl Methylthiomethyl Sulfoxide or + Dimethyl Sulfoxide at 298.15 K:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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