

# Hexadecanenitrile

<b>Other names:</b>	1-Cyanopentadecane Palmitic acid, nitrile Palmitonitrile palmitic acid nitrile
<b>Inchi:</b>	InChI=1S/C16H31N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h2-15H2,1H3
<b>InchiKey:</b>	WGXGAUQEMYSVJM-UHFFFAOYSA-N
<b>Formula:</b>	C16H31N
<b>SMILES:</b>	CCCCCCCCCCCCCCC#N
<b>Mol. weight [g/mol]:</b>	237.42
<b>CAS:</b>	629-79-8

## Physical Properties

Property code	Value	Unit	Source
gf	217.02	kJ/mol	Joback Method
hf	-208.69	kJ/mol	Joback Method
hfus	38.70	kJ/mol	Joback Method
hvap	93.30 ± 0.40	kJ/mol	NIST Webbook
log10ws	-6.39		Crippen Method
logp	5.991		Crippen Method
mcvol	237.680	ml/mol	McGowan Method
pc	1294.86	kPa	Joback Method
tb	606.20	K	NIST Webbook
tc	841.79	K	Joback Method
tf	304.55 ± 0.30	K	NIST Webbook
tf	304.66 ± 0.30	K	NIST Webbook
tf	304.55 ± 0.30	K	NIST Webbook
tf	302.15 ± 2.00	K	NIST Webbook
tf	304.15 ± 2.00	K	NIST Webbook
tf	304.00 ± 2.00	K	NIST Webbook
tf	304.15 ± 1.00	K	NIST Webbook
tf	302.65 ± 2.00	K	NIST Webbook
tf	300.00 ± 2.00	K	NIST Webbook
tf	306.15 ± 2.00	K	NIST Webbook
vc	0.958	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.09	J/molxK	696.60	Joback Method
cpg	758.39	J/molxK	841.79	Joback Method
cpg	744.91	J/molxK	812.75	Joback Method
cpg	730.76	J/molxK	783.71	Joback Method
cpg	715.93	J/molxK	754.67	Joback Method
cpg	700.38	J/molxK	725.64	Joback Method
cpg	667.04	J/molxK	667.56	Joback Method
hvapt	70.10	kJ/mol	555.50	NIST Webbook
pvap	0.01	kPa	376.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	8.26e-03	kPa	372.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	6.58e-03	kPa	369.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	379.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	382.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	5.32e-03	kPa	366.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	4.34e-03	kPa	363.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

pvap	3.42e-03	kPa	360.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	2.62e-03	kPa	357.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	2.12e-03	kPa	354.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.65e-03	kPa	351.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.28e-03	kPa	348.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	9.60e-04	kPa	345.10	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	524.20	K	13.30	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50542e+01

Coeff. B	-5.17314e+03
Coeff. C	-1.10494e+02
Temperature range (K), min.	460.82
Temperature range (K), max.	641.47

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles:</b>	<a href="https://www.doi.org/10.1016/j.jct.2004.08.004">https://www.doi.org/10.1016/j.jct.2004.08.004</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C629798&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C629798&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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