

Pentadecanenitrile

Other names:	1-tetradecyl cyanide Pentadecanitrile Pentadecanonitrile Tetradecyl cyanide n-Pentadecanonitrile
Inchi:	InChI=1S/C15H29N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16/h2-14H2,1H3
InchiKey:	KRKQHNVYOWTEQO-UHFFFAOYSA-N
Formula:	C15H29N
SMILES:	CCCCCCCCCCCCC#N
Mol. weight [g/mol]:	223.40
CAS:	18300-91-9

Physical Properties

Property code	Value	Unit	Source
gf	208.60	kJ/mol	Joback Method
hf	-188.05	kJ/mol	Joback Method
hfus	36.11	kJ/mol	Joback Method
hvap	59.46	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.601		Crippen Method
mcvol	223.590	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
tb	595.20	K	NIST Webbook
tc	819.33	K	Joback Method
tf	296.15 ± 2.00	K	NIST Webbook
vc	0.901	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.13	J/mol×K	644.68	Joback Method
cpg	628.71	J/mol×K	673.79	Joback Method
cpg	644.57	J/mol×K	702.90	Joback Method
cpg	659.70	J/mol×K	732.00	Joback Method

cpg	674.15	J/mol×K	761.11	Joback Method
cpg	687.93	J/mol×K	790.22	Joback Method
cpg	701.06	J/mol×K	819.33	Joback Method
pvap	2.19e-03	kPa	345.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.37e-03	kPa	339.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.76e-03	kPa	342.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.05e-03	kPa	336.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	2.87e-03	kPa	348.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	3.56e-03	kPa	351.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	4.59e-03	kPa	354.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	5.67e-03	kPa	357.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	7.04e-03	kPa	360.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

pvap	9.01e-03	kPa	363.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	366.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	369.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	372.10	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	1.48225e+01
Coeff. B	-4.98573e+03
Coeff. C	-1.06602e+02
Temperature range (K), min.	449.62
Temperature range (K), max.	630.81

Sources

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>

McGowan Method:

https://en.wikipedia.org/wiki/Joback_method

NIST Webbook:

<http://link.springer.com/article/10.1007/BF02311772>

The Yaws Handbook of Vapor Pressure:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C18300919&Units=SI>

Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

https://www.chemeo.com/doc/models/crippen_log10ws

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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