Tetradecanenitrile

Other names:	1-Cyanotridecane
	1-tridecanecarbonitrile
	Myristonitrile
	Myristyl nitrile
	Tetradecanonitrile
	tridecyl cyanide
Inchi:	InChI=1S/C14H27N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15/h2-13H2,1H3
InchiKey:	MLRCLPRHEOPXLL-UHFFFAOYSA-N
Formula:	C14H27N
SMILES:	CCCCCCCCCCCCCC#N
Mol. weight [g/mol]:	209.37
CAS:	629-63-0

Physical Properties

Property code	Value	Unit	Source
chl	-9107.70 ± 1.80	kJ/mol	NIST Webbook
gf	200.18	kJ/mol	Joback Method
hf	-174.80 ± 2.70	kJ/mol	NIST Webbook
hfl	-260.10 ± 2.60	kJ/mol	NIST Webbook
hfus	33.52	kJ/mol	Joback Method
hvap	85.30 ± 0.50	kJ/mol	NIST Webbook
hvap	85.29	kJ/mol	NIST Webbook
hvap	85.29 ± 0.51	kJ/mol	NIST Webbook
hvap	84.20 ± 0.20	kJ/mol	NIST Webbook
hvap	85.30	kJ/mol	NIST Webbook
log10ws	-5.55		Crippen Method
logp	5.211		Crippen Method
mcvol	209.500	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinpol	1698.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	285.95		NIST Webbook
rinpol	1695.00		NIST Webbook
tb	621.80	K	Joback Method
tc	797.24	K	Joback Method
tf	292.40 ± 0.30	K	NIST Webbook
tf	292.40 ± 0.30	K	NIST Webbook

tf	292.15 ± 1.00	K	NIST Webbook
tf	292.35 ± 1.00	K	NIST Webbook
tf	292.20 ± 2.00	K	NIST Webbook
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.56	J/mol×K	621.80	Joback Method
cpg	574.65	J/mol×K	651.04	Joback Method
cpg	590.02	J/mol×K	680.28	Joback Method
cpg	604.71	J/mol×K	709.52	Joback Method
cpg	618.74	J/mol×K	738.76	Joback Method
cpg	632.11	J/mol×K	768.00	Joback Method
cpg	644.87	J/mol×K	797.24	Joback Method
hvapt	71.40	kJ/mol	485.50	NIST Webbook
pvap	2.36e-03	kPa	336.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.39e-03	kPa	330.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.83e-03	kPa	333.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.09e-03	kPa	327.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	3.06e-03	kPa	339.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

pvap	3.83e-03	kPa	342.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	4.91e-03	kPa	345.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	6.28e-03	kPa	348.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	7.77e-03	kPa	351.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	9.82e-03	kPa	354.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	357.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	360.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	363.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	366.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.03	kPa	369.20	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	499.70	K	13.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44096e+01
Coeff. B	-4.74091e+03
Coeff. C	-1.02710e+02
Temperature range (K), min.	438.42
Temperature range (K), max.	623.79

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629630&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
McGowan 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
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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