Tridecanenitrile

Other names:	1-Cyanododecane
	dodecanecarbonitrile
	dodecyl cyanide
	n-Dodecyl cyanide
	tridecanonitrile
Inchi:	InChI=1S/C13H25N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14/h2-12H2,1H3
InchiKey:	WKJHMKQSIBMURP-UHFFFAOYSA-N
Formula:	C13H25N
SMILES:	CCCCCCCCCCCCC#N
Mol. weight [g/mol]:	195.34
CAS:	629-60-7

Physical Properties

Property code	Value	Unit	Source
gf	191.76	kJ/mol	Joback Method
hf	-146.77	kJ/mol	Joback Method
hfus	30.93	kJ/mol	Joback Method
hvap	80.30 ± 0.40	kJ/mol	NIST Webbook
log10ws	-5.13		Crippen Method
logp	4.821		Crippen Method
mcvol	195.410	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	1592.00		NIST Webbook
rinpol	270.65		NIST Webbook
tb	548.00 ± 5.00	K	NIST Webbook
tc	775.47	K	Joback Method
tf	282.85 ± 1.00	K	NIST Webbook
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.43	J/mol×K	598.92	Joback Method
cpg	521.97	J/mol×K	628.35	Joback Method

cpg	536.82	J/mol×K	657.77	Joback Method
cpg	551.01	J/mol×K	687.20	Joback Method
cpg	564.57	J/mol×K	716.62	Joback Method
cpg	577.50	J/mol×K	746.05	Joback Method
cpg	589.84	J/mol×K	775.47	Joback Method
hvapt	69.50	kJ/mol	473.00	NIST Webbook
pvap	2.80e-03	kPa	327.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	7.50e-04	kPa	313.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.20e-03	kPa	318.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	2.05e-03	kPa	324.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	2.40e-04	kPa	301.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	3.64e-03	kPa	330.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	4.66e-03	kPa	333.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	5.94e-03	kPa	336.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	7.54e-03	kPa	339.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

pvap	9.50e-03	kPa	342.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	345.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	348.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	351.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.02	kPa	354.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.03	kPa	357.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.03	kPa	360.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.04	kPa	363.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629607&Units=SI
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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume