Heptadecanenitrile

Other names:	1-cyanohexadecane
	Cetyl cyanide
	Heptadecanoic acid nitrile
	Margaronitrile
	heptadecanonitrile
	hexadecyl cyanide
Inchi:	InChI=1S/C17H33N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18/h2-16H2,1H3
InchiKey:	ZXPWFWWSCFIFII-UHFFFAOYSA-N
Formula:	C17H33N
SMILES:	CCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]:	251.45
CAS:	5399-02-0

Physical Properties

Property code	Value	Unit	Source
gf	225.44	kJ/mol	Joback Method
hf	-229.33	kJ/mol	Joback Method
hfus	41.29	kJ/mol	Joback Method
hvap	98.90 ± 0.40	kJ/mol	NIST Webbook
log10ws	-6.81		Crippen Method
logp	6.381		Crippen Method
mcvol	251.770	ml/mol	McGowan Method
pc	1209.83	kPa	Joback Method
rinpol	332.98		NIST Webbook
tb	690.44	K	Joback Method
tc	864.67	K	Joback Method
tf	307.15 ± 0.70	K	NIST Webbook
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.81	J/mol×K	864.67	Joback Method
cpg	803.02	J/mol×K	835.63	Joback Method

cpg	788.54	J/mol×K	806.59	Joback Method
cpg	773.34	J/mol×K	777.56	Joback Method
cpg	757.41	J/mol×K	748.52	Joback Method
cpg	740.70	J/mol×K	719.48	Joback Method
cpg	723.21	J/mol×K	690.44	Joback Method
hvapt	81.20	kJ/mol	522.50	NIST Webbook
pvap	3.16e-03	kPa	369.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	4.02e-03	kPa	372.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	2.52e-03	kPa	366.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	6.78e-03	kPa	379.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	8.24e-03	kPa	382.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	0.01	kPa	385.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	2.01e-03	kPa	363.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.56e-03	kPa	360.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	1.17e-03	kPa	357.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.

pvap	9.30e-04	kPa	354.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	7.20e-04	kPa	351.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	5.50e-04	kPa	348.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Linear Aliphatic Nitriles.
pvap	5.32e-03	kPa	376.20	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=C5399020&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
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