Octadecanenitrile

Other names:	1-Cyanoheptadecane
	Heptadecyl cyanide
	Nitril kyseliny stearove
	Octadecanonitrile
	Oktadekannitril
	Stearonitrile
Inchi:	InChI=1S/C18H35N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h2-17H2,1H3
InchiKey:	RHSBIGNQEIPSCT-UHFFFAOYSA-N
Formula:	C18H35N
SMILES:	CCCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]:	265.48
CAS:	638-65-3

Physical Properties

Property code	Value	Unit	Source
gf	233.86	kJ/mol	Joback Method
hf	-249.97	kJ/mol	Joback Method
hfus	43.88	kJ/mol	Joback Method
hvap	66.14	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.771		Crippen Method
mcvol	265.860	ml/mol	McGowan Method
pc	1132.91	kPa	Joback Method
rinpol	348.04		NIST Webbook
rinpol	348.04		NIST Webbook
tb	482.00 ± 3.00	K	NIST Webbook
tb	630.00 ± 4.00	K	NIST Webbook
tc	888.03	K	Joback Method
tf	314.65 ± 1.00	K	NIST Webbook
tf	314.39 ± 0.20	K	NIST Webbook
tf	313.85 ± 1.00	K	NIST Webbook
tf	314.03 ± 0.50	K	NIST Webbook
tf	314.03 ± 0.50	K	NIST Webbook
tf	315.65 ± 1.50	K	NIST Webbook
tf	315.65 ± 0.70	K	NIST Webbook
tf	312.15 ± 2.00	K	NIST Webbook
tf	315.90 ± 0.60	K	NIST Webbook

tf	314.15 ± 2.00	K	NIST Webbook
tf	314.15 ± 2.00	K	NIST Webbook
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.55	J/mol×K	713.32	Joback Method
cpg	798.48	J/mol×K	742.44	Joback Method
cpg	815.58	J/mol×K	771.56	Joback Method
cpg	831.89	J/mol×K	800.68	Joback Method
cpg	847.43	J/mol×K	829.80	Joback Method
cpg	862.23	J/mol×K	858.92	Joback Method
cpg	876.32	J/mol×K	888.03	Joback Method
hfust	56.50	kJ/mol	315.50	NIST Webbook
hvapt	78.60	kJ/mol	554.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	547.20	K	13.30	NIST Webbook
tbrp	466.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41565e+01
Coeff. B	-5.04688e+03
Coeff. C	-1.17722e+02
Temperature range (K), min.	481.62
Temperature range (K), max.	688.31

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C638653&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hfust:	Enthalpy of fusion at a given temperature
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