Hexanenitrile

Other names:	1-Cyanopentane
	1-pentanecarbonitrile
	CAPRONITRILE
	Hexanonitrile
	N-CAPRONITRILE
	NSC 1076
	PENTYL CYANIDE
	Tricapronile
	n-Amyl cyanide
	n-Caproic nitrile
	n-Pentyl cyanide
Inchi:	InChI=1S/C6H11N/c1-2-3-4-5-6-7/h2-5H2,1H3
InchiKey:	AILKHAQXUAOOFU-UHFFFAOYSA-N
Formula:	C6H11N
SMILES:	CCCCCC#N
Mol. weight [g/mol]:	97.16
CAS:	628-73-9

Physical Properties

Property code	Value	Unit	Source
af	0.5240		KDB
affp	806.00	kJ/mol	NIST Webbook
affp	804.60	kJ/mol	NIST Webbook
dm	3.50	debye	KDB
gf	132.82	kJ/mol	Joback Method
hf	-2.29	kJ/mol	Joback Method
hfus	12.80	kJ/mol	Joback Method
hvap	47.91 ± 0.10	kJ/mol	NIST Webbook
hvap	47.91	kJ/mol	NIST Webbook
hvap	47.70 ± 0.10	kJ/mol	NIST Webbook
hvap	47.90 ± 0.10	kJ/mol	NIST Webbook
hvap	49.10	kJ/mol	NIST Webbook
log10ws	-2.20		Crippen Method
logp	2.090		Crippen Method
mcvol	96.780	ml/mol	McGowan Method
pc	3242.40 ± 81.06	kPa	NIST Webbook
pc	3262.67 ± 81.06	kPa	NIST Webbook

pc	3300.00 ± 10.00	kPa	NIST Webbook
pc	3258.00 ± 81.06	kPa	NIST Webbook
pc	3300.00	kPa	KDB
pc	3252.53 ± 81.06	kPa	NIST Webbook
pc	3262.67 ± 81.06	kPa	NIST Webbook
rinpol	879.00		NIST Webbook
rinpol	874.60		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	874.60		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	795.50		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	884.00		NIST Webbook
ripol	1303.00		NIST Webbook
ripol	1303.00		NIST Webbook
ripol	1315.00		NIST Webbook
tb	436.00 ± 2.00	K	NIST Webbook
tb	433.00	K	NIST Webbook
tb	436.30 ± 0.60	K	NIST Webbook
tb	436.30 ± 0.40	K	NIST Webbook
tb	435.00 ± 3.00	K	NIST Webbook
tb	412.00 ± 6.00	K	NIST Webbook
tb	435.70 ± 3.00	K	NIST Webbook
tb	434.00 ± 3.00	K	NIST Webbook
tb	436.80	K	NIST Webbook
tb	435.70	K	NIST Webbook

tb	432.70 ± 7.00	K	NIST Webbook
tb	428.63 ± 3.00	K	NIST Webbook
tb	428.63 ± 0.50	K	NIST Webbook
tb	436.80	K	KDB
tb	437.10 ± 0.20	K	NIST Webbook
tb	434.70 ± 2.00	K	NIST Webbook
tb	437.20 ± 0.30	K	NIST Webbook
tb	436.47 ± 0.50	K	NIST Webbook
tb	432.70 ± 6.00	K	NIST Webbook
tc	633.80 ± 0.20	K	NIST Webbook
tc	621.80 ± 2.50	K	NIST Webbook
tc	622.05 ± 1.00	K	NIST Webbook
tc	621.75 ± 1.00	K	NIST Webbook
tc	633.80	K	KDB
tf	184.15 ± 1.50	K	NIST Webbook
tf	192.80	K	KDB
tf	228.15	K	NIST Webbook
tf	192.84 ± 0.05	K	NIST Webbook
tf	193.75 ± 1.00	K	NIST Webbook
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.86	J/mol×K	438.76	Joback Method
cpg	199.16	J/mol×K	470.25	Joback Method
cpg	208.06	J/mol×K	501.73	Joback Method
cpg	216.59	J/mol×K	533.22	Joback Method
cpg	224.75	J/mol×K	564.71	Joback Method
cpg	232.55	J/mol×K	596.19	Joback Method
cpg	240.01	J/mol×K	627.68	Joback Method
hvapt	43.30	kJ/mol	406.50	NIST Webbook
hvapt	44.60	kJ/mol	392.50	NIST Webbook
rhol	809.00	kg/m3	288.00	KDB

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46757e+01
Coeff. B	-3.74571e+03
Coeff. C	-6.25660e+01
Temperature range (K), min.	322.90
Temperature range (K), max.	462.57

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.96707e+01
Coeff. B	-6.37164e+03
Coeff. C	-3.39635e+00
Coeff. D	1.00064e-06
Temperature range (K), min.	192.85
Temperature range (K), max.	622.05

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1392
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1392
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
High pressure phase behavior for the binary mixture of valeronitrile, caprylonitrile and lauronitrile in supercritical carbon dioxide at temperatures from 313.2 to 393.2 K and pressures from 3.9 to 25.7 MPa:	https://www.doi.org/10.1016/j.fluid.2011.09.019
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C628739&Units=SI
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

Legend

af:	Acentric Factor
affp:	Proton affinity
cpg:	Ideal gas heat capacity
dm:	Dipole Moment

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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume