Isoamyl cyanide

Other names:	3-Methylbutyl cyanide
	4-Methylpentanenitrile
	4-Methylpentanonitrile
	4-Methylvaleronitrile
	ISO-CAPRONITRILE
	Isoamylkyanid
	Isocapronitrile
	Isopentyl cyanide
	NSC 6109
	Pentanenitrile, 4-methyl-
	Valeronitrile, 4-methyl-
Inchi:	InChI=1S/C6H11N/c1-6(2)4-3-5-7/h6H,3-4H2,1-2H3
InchiKey:	DUJMVKJJUANUMQ-UHFFFAOYSA-N
Formula:	C6H11N
SMILES:	CC(C)CCC#N
Mol. weight [g/mol]:	97.16
CAS:	542-54-1

Physical Properties

Property code	Value	Unit	Source
gf	130.38	kJ/mol	Joback Method
hf	-7.57	kJ/mol	Joback Method
hfus	9.28	kJ/mol	Joback Method
hvap	39.04	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.946		Crippen Method
mcvol	96.780	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	848.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	848.00		NIST Webbook
ripol	1253.00		NIST Webbook
tb	438.32	K	Joback Method

tc	631.63	K	Joback Method
tf	230.15 ± 5.00	K	NIST Webbook
tf	222.05 ± 0.30	K	NIST Webbook
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.99	J/mol×K	438.32	Joback Method
cpg	199.58	J/mol×K	470.54	Joback Method
cpg	208.77	J/mol×K	502.76	Joback Method
cpg	217.55	J/mol×K	534.97	Joback Method
cpg	225.93	J/mol×K	567.19	Joback Method
cpg	233.94	J/mol×K	599.41	Joback Method
cpg	241.57	J/mol×K	631.63	Joback Method
hvapt	35.70	kJ/mol	381.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51839e+01
Coeff. B	-3.80337e+03
Coeff. C	-5.98980e+01
Temperature range (K), min.	315.22
Temperature range (K), max.	445.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.46352e+01
Coeff. B	-4.29554e+03
Coeff. C	-2.78476e-04
Coeff. D	3.21228e-10
Temperature range (K), min.	332.15
Temperature range (K), max.	434.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C542541&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1393
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume