3-Butenenitrile

Other names:	1-Butene-4-nitrile
	3-Butenonitrile
	3-Butenylnitrile
	3-Cyano-1-propene
	3-Cyanopropene
	ALLYL CYANIDE
	ALLYLNITRILE
	Acetonitrile, vinyl-
	Allylkyanid
	BETA-BUTENONITRILE
	CH2=CHCH2CN
	NSC 2583
	Propene-3-nitrile
	TL 350
	VINYLACETONITRILE
	but-3-enenitrile
	«beta»-Butenonitrile
	Â«betaÂ»-Butenonitrile
Inchi:	InChI=1S/C4H5N/c1-2-3-4-5/h2H,1,3H2
InchiKey:	SJNALLRHIVGIBI-UHFFFAOYSA-N
Formula:	C4H5N
SMILES:	C=CCC#N
Mol. weight [g/mol]:	67.09
CAS:	109-75-1

Physical Properties

Property code	Value	Unit	Source
chl	-2405.00	kJ/mol	NIST Webbook
chl	-2406.40 ± 1.10	kJ/mol	NIST Webbook
gf	203.82	kJ/mol	Joback Method
hf	157.70	kJ/mol	NIST Webbook
hfl	117.70	kJ/mol	NIST Webbook
hfus	6.34	kJ/mol	Joback Method
hvap	40.00	kJ/mol	NIST Webbook
hvap	40.00	kJ/mol	NIST Webbook
hvap	40.00	kJ/mol	NIST Webbook
hvap	40.09	kJ/mol	NIST Webbook

ie	10.20 ± 0.02	eV	NIST Webbook
ie	10.18	eV	NIST Webbook
ie	10.55	eV	NIST Webbook
ie	10.22	eV	NIST Webbook
ie	10.39 ± 0.01	eV	NIST Webbook
log10ws	-1.22		Crippen Method
logp	1.086		Crippen Method
mcvol	64.300	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
rinpol	656.00		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	656.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	625.20		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	673.00		NIST Webbook
ripol	1186.00		NIST Webbook
ripol	1186.00		NIST Webbook
ripol	1186.00		NIST Webbook
ripol	1186.00		NIST Webbook
ripol	1186.00		NIST Webbook
tb	391.70	K	NIST Webbook
tb	391.57	K	KDB
tb	392.20	K	NIST Webbook
tb	391.00	K	NIST Webbook
tc	586.11	K	Joback Method
tf	198.07	K	Joback Method
vc	0.267	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	104.23	J/mol×K	389.68	Joback Method
cpg	109.84	J/mol×K	422.42	Joback Method
cpg	115.18	J/mol×K	455.16	Joback Method
cpg	120.26	J/mol×K	487.89	Joback Method
cpg	125.09	J/mol×K	520.63	Joback Method

cpg	129.68	J/mol×K	553.37	Joback Method
cpg	134.04	J/mol×K	586.11	Joback Method
hvapt	34.26	kJ/mol	391.70	NIST Webbook
hvapt	40.30	kJ/mol	355.00	NIST Webbook
hvapt	41.60	kJ/mol	323.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49868e+01
Coeff. B	-3.71208e+03
Coeff. C	-3.41820e+01
Temperature range (K), min.	286.72
Temperature range (K), max.	417.85

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.08663e+01
Coeff. B	-6.61192e+03
Coeff. C	-6.69232e+00
Coeff. D	3.86050e-06
Temperature range (K), min.	186.15
Temperature range (K), max.	584.00

Sources

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=1406
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
KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1406
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C109751&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
ie:	Ionization energy
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