2-Butenenitrile

Other names:	1-Cyano-1-propylene
	1-Cyanopropene
	1-Propenyl cyanide
	Croton acid nitrile
	Crotonic nitrile
	Crotonique nitrile
	Crotonitrile
	Crotonnitrile
	Crotononitrile
	NSC 165574
	cis or trans-crotononitrile
	trans or cis-crotononitrile
	«beta»-Methylacrylonitrile
	Â«betaÂ»-Methylacrylonitrile
Inchi:	InChI=1S/C4H5N/c1-2-3-4-5/h2-3H,1H3
InchiKey:	NKKMVIVFRUYPLQ-UHFFFAOYSA-N
Formula:	C4H5N
SMILES:	CC=CC#N
Mol. weight [g/mol]:	67.09
CAS:	4786-20-3

Physical Properties

Property code	Value	Unit	Source
gf	196.20	kJ/mol	Joback Method
hf	156.21	kJ/mol	Joback Method
hfus	7.82	kJ/mol	Joback Method
hvap	34.93	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.086		Crippen Method
mcvol	64.300	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
rinpol	664.00		NIST Webbook
rinpol	697.00		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	664.00		NIST Webbook

rinpol	619.80		NIST Webbook
rinpol	647.20		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	664.00		NIST Webbook
ripol	1162.00		NIST Webbook
ripol	1162.00		NIST Webbook
ripol	1162.00		NIST Webbook
tb	393.70	K	NIST Webbook
tc	599.62	K	Joback Method
tf	194.75	K	Joback Method
vc	0.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	102.51	J/mol×K	397.16	Joback Method
cpg	108.39	J/mol×K	430.90	Joback Method
cpg	113.94	J/mol×K	464.65	Joback Method
cpg	119.18	J/mol×K	498.39	Joback Method
cpg	124.11	J/mol×K	532.13	Joback Method
cpg	128.76	J/mol×K	565.87	Joback Method
cpg	133.16	J/mol×K	599.62	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46058e+01
Coeff. B	-3.42685e+03
Coeff. C	-5.05850e+01
Temperature range (K), min.	289.92
Temperature range (K), max.	419.29

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4786203&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
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