2,4-Pentadienenitrile

Other names:	1-Cyano-1,3-butadiene
	1-Cyanobutadiene
	1,3-Butadiene, 1-cyano-
	CH2=CHCH=CHCN
	penta-2,4-dienenitrile
Inchi:	InChI=1S/C5H5N/c1-2-3-4-5-6/h2-4H,1H2
InchiKey:	STSRVFAXSLNLLI-UHFFFAOYSA-N
Formula:	C5H5N
SMILES:	C=CC=CC#N
Mol. weight [g/mol]:	79.10
CAS:	1615-70-9

Physical Properties

Property code	Value	Unit	Source
gf	292.46	kJ/mol	Joback Method
hf	261.00	kJ/mol	Joback Method
hfus	9.13	kJ/mol	Joback Method
hvap	36.49	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.252		Crippen Method
mcvol	74.090	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
tb	416.72	K	Joback Method
tc	621.79	K	Joback Method
tf	204.26	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	122.01	J/mol×K	416.72	Joback Method
cpg	128.60	J/mol×K	450.90	Joback Method
cpg	134.77	J/mol×K	485.08	Joback Method
cpg	140.55	J/mol×K	519.26	Joback Method

cpg	145.97	J/mol×K	553.43	Joback Method
cpg	151.04	J/mol×K	587.61	Joback Method
cpg	155.79	J/mol×K	621.79	Joback Method

Sources

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=C1615709&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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