Methallyl cyanide

Other names:	3-Butenenitrile, 3-methyl-
	3-Methyl-3-butenenitrile
	3-Methyl-3-butenonitrile
	Methallylkyanid
	3-Methyl-3-butennitril
Inchi:	InChI=1S/C5H7N/c1-5(2)3-4-6/h1,3H2,2H3
InchiKey:	OIQDAVBXDLGCID-UHFFFAOYSA-N
Formula:	C5H7N
SMILES:	C=C(C)CC#N
Mol. weight [g/mol]:	81.12
CAS:	4786-19-0

Physical Properties

Property code	Value	Unit	Source
gf	203.69	kJ/mol	Joback Method
hf	133.99	kJ/mol	Joback Method
hfus	7.62	kJ/mol	Joback Method
hvap	36.61	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.476		Crippen Method
mcvol	78.390	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
tb	412.44	K	Joback Method
tc	611.25	K	Joback Method
tf	202.90 ± 0.60	K	NIST Webbook
vc	0.324	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.02	J/mol×K	412.44	Joback Method
cpg	145.29	J/mol×K	445.57	Joback Method
cpg	152.21	J/mol×K	478.71	Joback Method
cpg	158.78	J/mol×K	511.84	Joback Method

cpg	165.03	J/mol×K	544.98	Joback Method
cpg	170.97	J/mol×K	578.11	Joback Method
cpg	176.61	J/mol×K	611.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4786190&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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