Methylacrylonitrile

Other names:	.alpha.-methylacrylonitrile
	1-Methyl-1-cyanoethylene
	2-Cyano-1-propene
	2-Cyanopropene
	2-Cyanopropene-1
	2-Methyl-2-propenenitrile
	2-Methylacrylonitrile
	2-Methylpropenenitrile
	2-Propenenitrile, 2-methyl-
	ALPHA-METHACRYLONITRILE
	CH2C(CH3)CN
	ISOPROPENE CYANIDE
	ISOPROPENYLNITRILE
	METHACRYLONITRILE
	NSC 24145
	Propenenitrile, 2-methyl
	Rcra waste number U152
	USAF ST-40
	«alpha»-Methacrylonitrile
	«alpha»-Methylacrylonitrile
	Â«alphaÂ»-Methacrylonitrile
	Â«alphaÂ»-Methylacrylonitrile
Inchi:	InChI=1S/C4H5N/c1-4(2)3-5/h1H2,2H3
InchiKey:	GYCMBHHDWRMZGG-UHFFFAOYSA-N
Formula:	C4H5N
SMILES:	C=C(C)C#N
Mol. weight [g/mol]:	67.09
CAS:	126-98-7

Physical Properties

Property code	Value	Unit	Source
ea	0.01	eV	NIST Webbook
gf	195.27	kJ/mol	Joback Method
hf	154.63	kJ/mol	Joback Method
hfus	5.03	kJ/mol	Joback Method
hvap	34.39	kJ/mol	Joback Method

ie	10.34	eV	NIST Webbook
ie	10.37 ± 0.02	eV	NIST Webbook
ie	10.37 ± 0.05	eV	NIST Webbook
log10ws	-1.22		Crippen Method
logp	1.086		Crippen Method
mcvol	64.300	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
rinpol	575.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	574.90		NIST Webbook
rinpol	560.00		NIST Webbook
rinpol	560.00		NIST Webbook
rinpol	575.00		NIST Webbook
rinpol	575.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	614.00		NIST Webbook
tb	363.00 ± 3.00	K	NIST Webbook
tb	363.50	K	NIST Webbook
tc	590.11	K	Joback Method
tf	184.11	K	Joback Method
vc	0.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.36	J/mol×K	523.26	Joback Method
cpg	130.00	J/mol×K	556.68	Joback Method
cpg	104.25	J/mol×K	389.56	Joback Method
cpg	109.93	J/mol×K	422.98	Joback Method
cpg	115.34	J/mol×K	456.41	Joback Method
cpg	120.48	J/mol×K	489.83	Joback Method
cpg	134.39	J/mol×K	590.11	Joback Method
cpl	126.30	J/mol×K	298.15	NIST Webbook
hvapt	36.50	kJ/mol	323.00	NIST Webbook
hvapt	35.40	kJ/mol	296.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48730e+01
Coeff. B	-3.51409e+03
Coeff. C	-2.03170e+01
Temperature range (K), min.	237.35
Temperature range (K), max.	388.44

Sources

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
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1405
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126987&Units=SI

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
ea:	Electron affinity
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
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
tb:	Normal Boiling Point Temperature

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