3-Hexenedinitrile

Other names:	1,4-Dicyano butene-2
	1,4-Dicyano-2-butene
	1,4-Dicyano-2-butene,trans
	hex-3-enedinitrile
	trans-1,4-Dicyano-2-butene
	«beta»-Hydromuconononitrile
	Â«betaÂ»-Hydromuconononitrile
Inchi:	InChI=1S/C6H6N2/c7-5-3-1-2-4-6-8/h1-2H,3-4H2/b2-1+
InchiKey:	BSVZXPLUMFUWHW-OWOJBTEDSA-N
Formula:	C6H6N2
SMILES:	N#CCC=CCC#N
Mol. weight [g/mol]:	106.13
CAS:	1119-85-3

Physical Properties

Property code	Value	Unit	Source
gf	346.22	kJ/mol	Joback Method
hf	279.81	kJ/mol	Joback Method
hfus	14.51	kJ/mol	Joback Method
hvap	49.86	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.370		Crippen Method
mcvol	93.860	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
tb	545.00	K	Joback Method
tc	762.67	K	Joback Method
tf	282.28	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.83	J/mol×K	545.00	Joback Method
cpg	195.67	J/mol×K	581.28	Joback Method

cpg	202.08	J/mol×K	617.56	Joback Method
cpg	208.11	J/mol×K	653.83	Joback Method
cpg	213.78	J/mol×K	690.11	Joback Method
cpg	219.10	J/mol×K	726.39	Joback Method
cpg	224.12	J/mol×K	762.67	Joback Method
hvapt	49.40	kJ/mol	400.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	3.52704e+01
Coeff. B	-1.12773e+04
Coeff. C	-9.42670e+01
Temperature range (K), min.	416.63
Temperature range (K), max.	470.69

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1119853&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

hvapt: Enthalpy of vaporization at a given temperature

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume