Fumaronitrile

Other names:	2-Butenedinitrile, (E)-
	trans-1,2-Dicyanoethylene
	Fumaric nitrile
	Fumarodinitrile
	Furmaronitrile
	(E)-Butenedinitrile
	(E)-CH(CN)CH(CN)
	But-2-enedinitrile, (E)-
	(2E)-2-Butenedinitrile
	(E)-1,2-Dicyanoethylene
	2-Butenedinitrile, (2E)-
	NSC 17555
	trans-1,2-Dicyanoethene
Inchi:	InChI=1S/C4H2N2/c5-3-1-2-4-6/h1-2H/b2-1+
InchiKey:	KYPOHTVBFVELTG-OWOJBTEDSA-N
Formula:	C4H2N2
SMILES:	N#CC=CC#N
Mol. weight [g/mol]:	78.07
CAS:	764-42-1

Physical Properties

Property code	Value	Unit	Source
chs	-2128.00 ± 2.00	kJ/mol	NIST Webbook
ea	1.25 ± 0.09	eV	NIST Webbook
ea	0.79 ± 0.10	eV	NIST Webbook
gf	329.38	kJ/mol	Joback Method
hf	340.00 ± 3.00	kJ/mol	NIST Webbook
hfs	268.00 ± 2.00	kJ/mol	NIST Webbook
hfus	9.33	kJ/mol	Joback Method
hsub	68.60	kJ/mol	NIST Webbook
hsub	72.00 ± 0.80	kJ/mol	NIST Webbook
hsub	72.00	kJ/mol	NIST Webbook
hvap	45.41	kJ/mol	Joback Method
ie	11.16 ± 0.03	eV	NIST Webbook
ie	11.15	eV	NIST Webbook
ie	11.30	eV	NIST Webbook
log10ws	-1.08		Crippen Method

logp	0.590		Crippen Method
mcvol	65.680	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
tb	459.20	K	NIST Webbook
tc	724.59	K	Joback Method
tf	369.20 ± 0.80	K	NIST Webbook
tf	369.00 ± 3.00	K	NIST Webbook
vc	0.291	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.20	J/mol×K	649.47	Joback Method
cpg	128.23	J/mol×K	687.03	Joback Method
cpg	110.69	J/mol×K	499.24	Joback Method
cpg	114.72	J/mol×K	536.80	Joback Method
cpg	118.47	J/mol×K	574.36	Joback Method
cpg	121.95	J/mol×K	611.91	Joback Method
cpg	131.06	J/mol×K	724.59	Joback Method
hsubt	69.60	kJ/mol	259.50	NIST Webbook
hsubt	72.00 ± 0.80	kJ/mol	263.00	NIST Webbook

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=C764421&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
ea: Electron affinity

gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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