Tetracyanoethylene

Other names:	Ethenetetracarbonitrile «delta»2,2'-Bimalononitrile Ethene, tetracyano- Ethylenetetracarbonitrile Tetracyanoethene TCNE (NC)2CC(CN)2 Tetrakyanethylen 1,1,2,2-Tetracyanoethene 1,1,2,2-Tetracyanoethylene Ethylene, tetracyano- 1,1,2,2-Ethenetetracarbonitrile NSC 24833
Inchi:	InChI=1S/C6N4/c7-1-5(2-8)6(3-9)4-10
InchiKey:	NLDYACGHTUPAQU-UHFFFAOYSA-N
Formula:	C6N4
SMILES:	N#CC(C#N)=C(C#N)C#N
Mol. weight [g/mol]:	128.09
CAS:	670-54-2

Physical Properties

Property code	Value	Unit	Source
chs	-2996.00 ± 2.00	kJ/mol	NIST Webbook
chs	-3033.30	kJ/mol	NIST Webbook
chs	-2985.00 ± 2.00	kJ/mol	NIST Webbook
ea	2.03 ± 0.05	eV	NIST Webbook
ea	3.17 ± 0.20	eV	NIST Webbook
ea	2.88 ± 0.06	eV	NIST Webbook
ea	3.16 ± 0.02	eV	NIST Webbook
ea	2.30 ± 0.30	eV	NIST Webbook
ea	1.70 ± 0.30	eV	NIST Webbook
gf	595.48	kJ/mol	Joback Method
hf	705.00 ± 6.30	kJ/mol	NIST Webbook
hf	714.00	kJ/mol	NIST Webbook
hf	688.10	kJ/mol	NIST Webbook
hfs	633.00 ± 2.00	kJ/mol	NIST Webbook
hfs	624.00 ± 2.00	kJ/mol	NIST Webbook

hfs	607.10	kJ/mol	NIST Webbook
hfus	14.90	kJ/mol	Joback Method
hsub	81.00	kJ/mol	NIST Webbook
hsub	81.20	kJ/mol	NIST Webbook
hvap	70.98	kJ/mol	Joback Method
ie	11.67 ± 0.02	eV	NIST Webbook
ie	11.77 ± 0.01	eV	NIST Webbook
ie	11.79 ± 0.05	eV	NIST Webbook
log10ws	-1.65		Crippen Method
logp	0.377		Crippen Method
mcvol	96.620	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
tb	496.20	K	NIST Webbook
tc	1000.10	K	Joback Method
tf	472.00 ± 0.20	K	NIST Webbook
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.61	J/mol×K	790.78	Joback Method
cpg	193.51	J/mol×K	832.65	Joback Method
cpg	196.23	J/mol×K	874.51	Joback Method
cpg	198.81	J/mol×K	916.38	Joback Method
cpg	201.28	J/mol×K	958.24	Joback Method
cpg	187.48	J/mol×K	748.92	Joback Method
cpg	203.68	J/mol×K	1000.10	Joback Method
hfust	24.92	kJ/mol	472.20	NIST Webbook
hfust	24.92	kJ/mol	472.20	NIST Webbook
hsubt	81.40	kJ/mol	352.00	NIST Webbook
hsubt	84.30	kJ/mol	301.00	NIST Webbook
hsubt	81.20 ± 5.90	kJ/mol	350.00	NIST Webbook

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=C670542&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature
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