Cyano radical

Inchi: InChI=1S/CN/c1-2
InchiKey: JEVCWSUVFOYBFI-UHFFFAOYSA-N
Formula: CN
SMILES: [C]#N
Mol. weight [g/mol]: 26.02
CAS: 2074-87-5

Physical Properties

Property code	Value	Unit	Source
ea	5.64 ± 0.20	eV	NIST Webbook
ea	3.83 ± 0.09	eV	NIST Webbook
ea	2.80 ± 0.02	eV	NIST Webbook
ea	3.86 ± 0.01	eV	NIST Webbook
ea	3.16	eV	NIST Webbook
ea	2.78	eV	NIST Webbook
ea	3.82 ± 0.02	eV	NIST Webbook
gf	143.10	kJ/mol	Joback Method
hf	156.72	kJ/mol	Joback Method
hfpi	1750.00 ± 4.00	kJ/mol	NIST Webbook
hfus	1.53	kJ/mol	Joback Method
hvap	28.15	kJ/mol	Joback Method
ie	14.20 ± 0.02	eV	NIST Webbook
ie	14.17	eV	NIST Webbook
ie	13.60	eV	NIST Webbook
ie	14.20 ± 0.30	eV	NIST Webbook
ie	14.03 ± 0.02	eV	NIST Webbook
ie	14.50 ± 0.20	eV	NIST Webbook
log10ws	0.28		Crippen Method
logp	0.096		Crippen Method
mcvol	24.180	ml/mol	McGowan Method
pc	5962.94	kPa	Joback Method
tb	323.66	K	Joback Method
tc	514.23	K	Joback Method
tf	182.39	K	Joback Method
vc	0.108	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	24.62	J/mol×K	323.66	Joback Method
cpg	25.63	J/mol×K	355.42	Joback Method
cpg	26.44	J/mol×K	387.18	Joback Method
cpg	27.08	J/mol×K	418.95	Joback Method
cpg	27.56	J/mol×K	450.71	Joback Method
cpg	27.91	J/mol×K	482.47	Joback Method
cpg	28.13	J/mol×K	514.23	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2074875&Units=SI
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

Legend

cpg: Ideal gas heat capacity
ea: Electron affinity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfpi: Enthalpy of formation of positive ion at standard conditions
hfus: Enthalpy of fusion at standard conditions
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