Cyanomethyl radical

Inchi: InChI=1S/C2H2N/c1-2-3/h1H2
InchiKey: XSTKDMFTWATIQP-UHFFFAOYSA-N
Formula: C2H2N
SMILES: [CH2]C#N
Mol. weight [g/mol]: 40.04
CAS: 2932-82-3

Physical Properties

Property code	Value	Unit	Source
ea	1.54 ± 0.01	eV	NIST Webbook
ea	1.59 ± 0.13	eV	NIST Webbook
ea	1.56 ± 0.01	eV	NIST Webbook
ea	1.51 ± 0.02	eV	NIST Webbook
ea	1.60 ± 0.20	eV	NIST Webbook
ea	1.53 ± 0.01	eV	NIST Webbook
gf	151.52	kJ/mol	Joback Method
hf	136.08	kJ/mol	Joback Method
hfus	4.12	kJ/mol	Joback Method
hvap	30.38	kJ/mol	Joback Method
ie	10.90 ± 0.10	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	9.90 ± 0.10	eV	NIST Webbook
ie	10.30 ± 0.02	eV	NIST Webbook
log10ws	-0.14		Crippen Method
logp	0.344		Crippen Method
mcvol	38.270	ml/mol	McGowan Method
pc	5168.28	kPa	Joback Method
tb	346.54	K	Joback Method
tc	536.93	K	Joback Method
tf	193.66	K	Joback Method
vc	0.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	51.34	J/mol×K	346.54	Joback Method
cpg	54.12	J/mol×K	378.27	Joback Method
cpg	56.64	J/mol×K	410.00	Joback Method
cpg	58.91	J/mol×K	441.73	Joback Method
cpg	60.96	J/mol×K	473.47	Joback Method
cpg	62.81	J/mol×K	505.20	Joback Method
cpg	64.49	J/mol×K	536.93	Joback Method

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=C2932823&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas 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
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