cyanogen iodide

Inchi: InChI=1S/CIN/c2-1-3
InchiKey: WPBXOELOQKLBDF-UHFFFAOYSA-N
Formula: CIN
SMILES: N#CI
Mol. weight [g/mol]: 152.92
CAS: 506-78-5

Physical Properties

Property code	Value	Unit	Source
gf	148.84	kJ/mol	Joback Method
hf	224.60 ± 4.30	kJ/mol	NIST Webbook
hfs	164.80 ± 4.30	kJ/mol	NIST Webbook
hfus	4.26	kJ/mol	Joback Method
hsub	59.90 ± 0.20	kJ/mol	NIST Webbook
hsub	59.83 ± 0.42	kJ/mol	NIST Webbook
hvap	40.00 ± 0.30	kJ/mol	NIST Webbook
ie	10.91 ± 0.02	eV	NIST Webbook
ie	10.91	eV	NIST Webbook
ie	10.87 ± 0.00	eV	NIST Webbook
ie	10.87 ± 0.02	eV	NIST Webbook
log10ws	-1.55		Crippen Method
logp	0.902		Crippen Method
mcvol	52.150	ml/mol	McGowan Method
pc	5398.63	kPa	Joback Method
tb	417.50	K	Joback Method
tc	657.23	K	Joback Method
tf	224.08	K	Joback Method
vc	0.205	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	52.69	J/mol×K	617.27	Joback Method
cpg	49.36	J/mol×K	417.50	Joback Method

cpg	50.21	J/mol×K	457.45	Joback Method
cpg	50.96	J/mol×K	497.41	Joback Method
cpg	51.62	J/mol×K	537.36	Joback Method
cpg	52.19	J/mol×K	577.32	Joback Method
cpg	53.13	J/mol×K	657.23	Joback Method
hsubt	59.80 ± 0.40	kJ/mol	381.50	NIST Webbook
hsubt	59.90	kJ/mol	381.50	NIST Webbook
hsubt	58.60	kJ/mol	356.00	NIST Webbook
hsubt	58.30	kJ/mol	326.00	NIST Webbook
hvapt	40.00	kJ/mol	422.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58763e+01
Coeff. B	-4.81263e+03
Temperature range (K), min.	308.73
Temperature range (K), max.	455.53

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=C506785&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

Legend

cpg:	Ideal gas heat capacity
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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

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