

# 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	10.87 ± 0.02	eV	NIST Webbook
ie	10.87 ± 0.00	eV	NIST Webbook
ie	10.91	eV	NIST Webbook
ie	10.91 ± 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	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	52.69	J/mol×K	617.27	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	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58763e+01
Coeff. B	-4.81263e+03
Temperature range (K), min.	308.73
Temperature range (K), max.	455.53

## Sources

The Yaws Handbook of Vapor Pressure:  
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>  
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Joback Method:

[https://en.wikipedia.org/wiki/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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions

<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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