3-Iodobenzonitrile

Other names:	3-cyanoiodobenzene
	3-cyanophenyl iodide
	m-cyanoiodobenzene
	m-iodobenzonitrile
Inchi:	InChI=1S/C7H4IN/c8-7-3-1-2-6(4-7)5-9/h1-4H
InchiKey:	BGARPMGQRREXLN-UHFFFAOYSA-N
Formula:	C7H4IN
SMILES:	N#Cc1cccc(I)c1
Mol. weight [g/mol]:	229.02
CAS:	69113-59-3

Physical Properties

Property code	Value	Unit	Source
gf	302.14	kJ/mol	Joback Method
hf	279.00	kJ/mol	Joback Method
hfus	13.45	kJ/mol	Joback Method
hvap	53.97	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.163		Crippen Method
mcvol	112.930	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
tb	586.44	K	Joback Method
tc	857.62	K	Joback Method
tf	313.27	K	Thermodynamic and aromaticity studies for the assessment of the halogen...cyano interactions on Iodobenzonitrile
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.95	J/mol×K	586.44	Joback Method

cpg	202.63	J/mol×K	631.64	Joback Method
cpg	209.62	J/mol×K	676.83	Joback Method
cpg	215.97	J/mol×K	722.03	Joback Method
cpg	221.74	J/mol×K	767.23	Joback Method
cpg	226.99	J/mol×K	812.42	Joback Method
cpg	231.79	J/mol×K	857.62	Joback Method

Sources

Thermodynamic and aromaticity studies for the assessment of the halogen···cyano interactions on iodobenzonitrile:	https://www.doi.org/10.1016/j.jct.2013.06.003
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=C69113593&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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