1,3-Dicyanobenzene

Other names:	1,3-Benzenedicarbonitrile
	Isophthalonitrile
	m-Benzenedinitrile
	m-Dicyanobenzene
	3-Cyanobenzonitrile
	Isophthalodinitrile
	Isoftalodinitril
	Isophtalonitrile
	IPN
	Nitril kyseliny isoftalove
	1,3-Benzodinitrile
	1,3-Benzendikarbonitril
	Dinitrile of isophthalic acid
	Isoftalonitril
	m-Phthalodinitrile
	m-Cyanobenzonitrile
	NSC 87880
	benzene-1,3-dicarbonitrile
Inchi:	InChI=1S/C8H4N2/c9-5-7-2-1-3-8(4-7)6-10/h1-4H
InchiKey:	LAQPNDIUHRHNCV-UHFFFAOYSA-N
Formula:	C8H4N2
SMILES:	N#Cc1cccc(C#N)c1
Mol. weight [g/mol]:	128.13
CAS:	626-17-5

Physical Properties

Property code	Value	Unit	Source
affp	779.30	kJ/mol	NIST Webbook
basg	750.40	kJ/mol	NIST Webbook
chs	-3992.29 ± 0.75	kJ/mol	NIST Webbook
ea	0.91 ± 0.10	eV	NIST Webbook
gf	385.62	kJ/mol	Joback Method
hf	362.70 ± 2.00	kJ/mol	NIST Webbook
hfs	272.60 ± 1.30	kJ/mol	NIST Webbook
hfus	13.14	kJ/mol	Joback Method
hsub	90.10 ± 1.50	kJ/mol	NIST Webbook
hsub	90.10	kJ/mol	NIST Webbook

hsub	90.10 ± 1.50	kJ/mol	NIST Webbook
hvap	57.30	kJ/mol	Joback Method
ie	10.60	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
log10ws	-2.18		Crippen Method
logp	1.430		Crippen Method
mcvol	102.580	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
tb	618.26	K	Joback Method
tc	866.90	K	Joback Method
tf	348.84	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.21	J/mol×K	618.26	Joback Method
cpg	220.77	J/mol×K	659.70	Joback Method
cpg	227.75	J/mol×K	701.14	Joback Method
cpg	234.16	J/mol×K	742.58	Joback Method
cpg	240.06	J/mol×K	784.02	Joback Method
cpg	245.45	J/mol×K	825.46	Joback Method
cpg	250.39	J/mol×K	866.90	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=C626175&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp: Proton affinity

basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
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