1,2-Benzenedicarbonitrile

Other names:	1,2-Benzendikarbonitril
	1,2-Benzodinitrile
	1,2-Dicyanobenzene
	Ftalodinitril
	Ftalonitril
	NSC 17562
	Phthalic acid dinitrile
	Phthalodinitrile
	Phthalonitrile
	USAF ND-09
	o-Benzenedicarbonitrile
	o-Benzenedinitrile
	o-Cyanobenzonitrile
	o-Dicyanobenzene
	o-PDN
	o-Phthalodinitrile
Inchi:	InChI=1S/C8H4N2/c9-5-7-3-1-2-4-8(7)6-10/h1-4H
InchiKey:	XQZYPMVTSDWCCE-UHFFFAOYSA-N
Formula:	C8H4N2
SMILES:	N#Cc1ccccc1C#N
Mol. weight [g/mol]:	128.13
CAS:	91-15-6

Physical Properties

Property code	Value	Unit	Source
chs	-4000.36 ± 0.67	kJ/mol	NIST Webbook
chs	-3994.90	kJ/mol	NIST Webbook
ea	0.95 ± 0.09	eV	NIST Webbook
ea	1.11 ± 0.13	eV	NIST Webbook
gf	385.62	kJ/mol	Joback Method
hf	362.00	kJ/mol	NIST Webbook
hf	368.30	kJ/mol	NIST Webbook
hf	367.50 ± 1.90	kJ/mol	NIST Webbook
hfs	275.10	kJ/mol	NIST Webbook
hfs	281.40 ± 1.90	kJ/mol	NIST Webbook
hfs	280.60 ± 1.20	kJ/mol	NIST Webbook
hfus	13.14	kJ/mol	Joback Method

hsub	86.90 ± 1.50	kJ/mol	NIST Webbook
hsub	86.90	kJ/mol	NIST Webbook
hsub	86.90 ± 1.50	kJ/mol	NIST Webbook
hvap	57.30	kJ/mol	Joback Method
ie	9.90	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	10.27	eV	NIST Webbook
log10ws	-2.38		Aqueous Solubility Prediction Method
log10ws	-2.38		Estimated Solubility Method
logp	1.430		Crippen Method
mcvol	102.580	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	1304.00		NIST Webbook
rinpol	1304.00		NIST Webbook
ss	192.40	J/mol×K	NIST Webbook
ss	192.40	J/mol×K	NIST Webbook
tb	618.26	K	Joback Method
tc	866.90	K	Joback Method
tf	413.05 ± 0.20	K	NIST Webbook
tf	412.92 ± 0.25	K	NIST Webbook
tf	414.00	K	NIST Webbook
tt	414.00 ± 0.10	K	NIST Webbook
tt	414.00 ± 0.20	K	NIST Webbook
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.39	J/mol×K	866.90	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	213.21	J/mol×K	618.26	Joback Method
cps	161.30	J/mol×K	298.15	NIST Webbook
cps	161.30	J/mol×K	298.15	NIST Webbook
hfust	20.00	kJ/mol	414.00	NIST Webbook
hfust	20.00	kJ/mol	414.00	NIST Webbook

hfust	20.00	kJ/mol	414.10	NIST Webbook
hfust	20.00	kJ/mol	414.10	NIST Webbook
sfust	48.26	J/mol×K	414.00	NIST Webbook
sfust	48.26	J/mol×K	414.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	424.00 ± 1.00	K	1.30	NIST Webbook

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C91156&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase 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
hfust: Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume