1,4-Benzenedicarbonitrile

Other names:	Terephthalonitrile
	p-Benzenedinitrile
	p-Dicyanobenzene
	p-Phthalodinitrile
	Terephthalic acid dinitrile
	Terephthalodinitrile
	1,4-Dicyanobenzene
	4-Cyanobenzonitrile
	Terephthalonitrile (di)
	p-Pdn
	Nitril kyseliny tereftalove
	Tereftalodinitril
	1,4-Benzodinitrile
	1,4-Benzendikarbonitril
	Tereftalonitril
	p-Phthalonitrile
	p-Cyanobenzonitrile
	NSC 144977
	NSC 78439
Inchi:	InChI=1S/C8H4N2/c9-5-7-1-2-8(6-10)4-3-7/h1-4H
InchiKey:	BHXFKXOIODIUJO-UHFFFAOYSA-N
Formula:	C8H4N2
SMILES:	N#Cc1ccc(C#N)cc1
Mol. weight [g/mol]:	128.13
CAS:	623-26-7

Physical Properties

Property code	Value	Unit	Source
affp	779.00	kJ/mol	NIST Webbook
basg	751.80	kJ/mol	NIST Webbook
chs	-3988.20 ± 0.60	kJ/mol	NIST Webbook
chs	-3988.04 ± 0.59	kJ/mol	NIST Webbook
ea	1.09 ± 0.09	eV	NIST Webbook
gf	385.62	kJ/mol	Joback Method
hf	358.30 ± 2.20	kJ/mol	NIST Webbook
hf	357.10 ± 1.90	kJ/mol	NIST Webbook
hfs	268.50 ± 1.20	kJ/mol	NIST Webbook

hfs	268.30 ± 1.20	kJ/mol	NIST Webbook
hfus	13.14	kJ/mol	Joback Method
hvap	57.30	kJ/mol	Joback Method
ie	10.10	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	10.10	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
ss	183.00	J/mol×K	NIST Webbook
tb	618.26	K	Joback Method
tc	866.90	K	Joback Method
tf	348.84	K	Joback Method
tt	450.15 ± 1.00	K	NIST Webbook
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
cps	161.20	J/mol×K	298.15	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C623267&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume