Benzonitrile, 4-bromo-

Other names:	1-Bromo-4-cyanobenzene
	4-Bromobenzoic acid nitrile
	4-bromobenzonitrile
	4-bromocyanobenzene
	4-cyanophenyl bromide
	Benzonitrile, p-bromo-
	p-Bromophenyl cyanide
	p-bromobenzonitrile
	p-bromocyanobenzene
	p-cyanophenyl bromide
Inchi:	InChI=1S/C7H4BrN/c8-7-3-1-6(5-9)2-4-7/h1-4H
InchiKey:	HQSCPPCMBMFJJN-UHFFFAOYSA-N
Formula:	C7H4BrN
SMILES:	N#Cc1ccc(Br)cc1
Mol. weight [g/mol]:	182.02
CAS:	623-00-7

Physical Properties

Property code	Value	Unit	Source
gf	258.34	kJ/mol	Joback Method
hf	228.46	kJ/mol	Joback Method
hfus	14.33	kJ/mol	Joback Method
hvap	51.03	kJ/mol	Joback Method
ie	9.54	eV	NIST Webbook
ie	9.90 ± 0.05	eV	NIST Webbook
log10ws	-2.99		Crippen Method
logp	2.321		Crippen Method
mcvol	104.610	ml/mol	McGowan Method
pc	4271.86	kPa	Joback Method
tb	509.00 ± 1.00	K	NIST Webbook
tb	509.20	K	NIST Webbook
tc	812.58	K	Joback Method
tf	384.30	K	Thermodynamic and aromaticity studies for the assessment of the halogen...cyano interactions on Iodobenzonitrile

tf	386.60	K	NIST Webbook
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.17	J/mol×K	559.46	Joback Method
cpg	195.99	J/mol×K	601.65	Joback Method
cpg	203.16	J/mol×K	643.83	Joback Method
cpg	209.74	J/mol×K	686.02	Joback Method
cpg	215.77	J/mol×K	728.21	Joback Method
cpg	221.29	J/mol×K	770.39	Joback Method
cpg	226.35	J/mol×K	812.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.00	K	1.70	NIST Webbook

Sources

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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=C623007&Units=SI

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume