Benzonitrile, 3-bromo-

Other names:	1-Bromo-3-cyanobenzene
	3-Bromobenzoic acid nitrile
	3-bromobenzonitrile
	3-cyanophenyl bromide
	Benzonitrile, m-bromo-
	NSC 59731
	m-bromobenzonitrile
Inchi:	InChI=1S/C7H4BrN/c8-7-3-1-2-6(4-7)5-9/h1-4H
InchiKey:	STXAVEHFKAXGOX-UHFFFAOYSA-N
Formula:	C7H4BrN
SMILES:	N#Cc1cccc(Br)c1
Mol. weight [g/mol]:	182.02
CAS:	6952-59-6

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
log10ws	-2.99		Crippen Method
logp	2.321		Crippen Method
mcvol	104.610	ml/mol	McGowan Method
pc	4271.86	kPa	Joback Method
tb	498.00	K	NIST Webbook
tb	498.20	K	NIST Webbook
tc	812.58	K	Joback Method
tf	311.50 ± 0.50	K	NIST Webbook
tf	312.65	K	Thermodynamic and aromaticity studies for the assessment of the halogen...cyano interactions on Iodobenzonitrile
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	391.60	K	2.70	NIST Webbook

Sources

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=C6952596&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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