Benzenamine, 4-bromo-

Other names:	Aniline, p-bromo-
	p-Bromoaniline
	p-Bromophenylamine
	4-Bromoaniline
	4-Bromanilinu
Inchi:	InChI=1S/C6H6BrN/c7-5-1-3-6(8)4-2-5/h1-4H,8H2
InchiKey:	WDFQBORIUYODSI-UHFFFAOYSA-N
Formula:	C6H6BrN
SMILES:	Nc1ccc(Br)cc1
Mol. weight [g/mol]:	172.02
CAS:	106-40-1

Physical Properties

Property code	Value	Unit	Source
gf	183.19	kJ/mol	Joback Method
hf	118.01	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hsub	79.40 ± 1.70	kJ/mol	NIST Webbook
hvap	48.96	kJ/mol	Joback Method
ie	7.70 ± 0.10	eV	NIST Webbook
log10ws	-2.27		Crippen Method
logp	2.031		Crippen Method
mcvol	99.120	ml/mol	McGowan Method
pc	5470.75	kPa	Joback Method
rinpol	1248.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1245.00		NIST Webbook
tb	492.90 ± 0.60	K	NIST Webbook
tc	757.06	K	Joback Method
tf	339.38	K	Joback Method
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.74	J/mol×K	507.03	Joback Method
cpg	188.96	J/mol×K	548.70	Joback Method
cpg	197.46	J/mol×K	590.37	Joback Method
cpg	205.28	J/mol×K	632.05	Joback Method
cpg	212.48	J/mol×K	673.72	Joback Method
cpg	219.10	J/mol×K	715.39	Joback Method
cpg	225.18	J/mol×K	757.06	Joback Method
hfust	16.75	kJ/mol	336.00	NIST Webbook
hfust	13.36	kJ/mol	336.00	NIST Webbook

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=C106401&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
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

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume