Benzenamine, 3-bromo-

Other names:	Aniline, m-bromo-
	m-Aminobromobenzene
	m-Bromoaniline
	3-Bromoaniline
	Aniline, 3-bromo-
	3-BrC6H4NH2
Inchi:	InChI=1S/C6H6BrN/c7-5-2-1-3-6(8)4-5/h1-4H,8H2
InchiKey:	DHYHYLGCQVVLOQ-UHFFFAOYSA-N
Formula:	C6H6BrN
SMILES:	Nc1cccc(Br)c1
Mol. weight [g/mol]:	172.02
CAS:	591-19-5

Physical Properties

Property code	Value	Unit	Source
affp	873.20	kJ/mol	NIST Webbook
basg	841.40	kJ/mol	NIST Webbook
gf	183.19	kJ/mol	Joback Method
hf	118.01	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	63.40 ± 1.50	kJ/mol	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	1250.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1250.20		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1242.00		NIST Webbook
tb	524.00	K	NIST Webbook
tb	524.20	K	NIST Webbook
tc	757.06	K	Joback Method
tf	291.60	K	NIST Webbook
tf	289.80	K	NIST Webbook
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	14.68	kJ/mol	291.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.20	K	1.60	NIST Webbook
tbrp	403.00	K	1.60	NIST Webbook

Sources

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=C591195&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume