Benzenamine, 2-bromo-

Other names:	Aniline, o-bromo-
	o-Aminobromobenzene
	o-Bromoaniline
	2-Bromoaniline
Inchi:	InChI=1S/C6H6BrN/c7-5-3-1-2-4-6(5)8/h1-4H,8H2
InchiKey:	AOPBDRUWRLBSDB-UHFFFAOYSA-N
Formula:	C6H6BrN
SMILES:	Nc1ccccc1Br
Mol. weight [g/mol]:	172.02
CAS:	615-36-1

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	75.00 ± 1.40	kJ/mol	NIST Webbook
hvap	48.96	kJ/mol	Joback Method
ie	8.45	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	1178.50		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1178.50		NIST Webbook
tb	502.00	K	NIST Webbook
tb	502.20	K	NIST Webbook
tc	757.06	K	Joback Method
tf	305.00	K	NIST Webbook
tf	301.80	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	16.14	kJ/mol	304.10	NIST Webbook
hfust	20.04	kJ/mol	305.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	412.50 ± 1.50	K	6.75	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=C615361&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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