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]: 172.03

Physical Properties

Property code	Value	Unit	Source
af	0.4351		Cheméo Relay (1.0)
affp	873.20	kJ/mol	NIST Webbook
basg	841.40	kJ/mol	NIST Webbook
gf	183.19	kJ/mol	Joback Method
hf	127.00	kJ/mol	Cheméo Relay (1.0)
hfus	15.43	kJ/mol	Joback Method
hvap	63.40 ± 1.50	kJ/mol	NIST Webbook
ie	8.10	eV	Cheméo Relay (1.0)
log10ws	-1.77		Cheméo Relay (1.0)
logp	2.031		Crippen Method
mcvol	99.120	ml/mol	McGowan Method
pc	5470.75	kPa	Joback Method
rinpol	1250.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1250.20		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1295.00		NIST Webbook
tb	524.00	K	NIST Webbook
tb	524.20	K	NIST Webbook
tc	777.84	K	Cheméo Relay (1.0)
tf	289.80	K	NIST Webbook
tf	291.60	K	NIST Webbook

vc	0.342	m3/kmol	Cheméo Relay (1.0)

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C591195&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
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