4-Bromo-3-chloroaniline

Other names: Benzenamine, 4-bromo-3-chloro-
Aniline, 4-bromo-3-chloro
Inchi: InChI=1S/C6H5BrClN/c7-5-2-1-4(9)3-6(5)8/h1-3H,9H2
InchiKey: QLYHPNUFNZJXOQ-UHFFFAOYSA-N
Formula: C6H5BrClN
SMILES: Nc1ccc(Br)c(Cl)c1
Mol. weight [g/mol]: 206.47
CAS: 21402-26-6

Physical Properties

Property code	Value	Unit	Source
gf	161.63	kJ/mol	Joback Method
hf	90.80	kJ/mol	Joback Method
hfus	19.24	kJ/mol	Joback Method
hvap	54.01	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.685		Crippen Method
mcvol	111.360	ml/mol	McGowan Method
pc	5073.01	kPa	Joback Method
rinpol	1468.00		NIST Webbook
tb	549.44	K	Joback Method
tc	805.41	K	Joback Method
tf	381.82	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.79	J/mol×K	549.44	Joback Method
cpg	206.83	J/mol×K	592.10	Joback Method
cpg	214.23	J/mol×K	634.76	Joback Method
cpg	221.04	J/mol×K	677.42	Joback Method
cpg	227.30	J/mol×K	720.08	Joback Method
cpg	233.04	J/mol×K	762.74	Joback Method

cpg	238.31	J/mol×K	805.41	Joback Method

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=C21402266&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume