4-Bromo-3-nitroaniline

Other names: Benzenamine, 4-bromo-3-nitro-
Inchi: InChI=1S/C6H5BrN2O2/c7-5-2-1-4(8)3-6(5)9(10)11/h1-3H,8H2
InchiKey: PITHQPMZWKZGRZ-UHFFFAOYSA-N
Formula: C6H5BrN2O2
SMILES: Nc1ccc(Br)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 217.02
CAS: 53324-38-2

Physical Properties

Property code	Value	Unit	Source
gf	209.11	kJ/mol	Joback Method
hf	95.78	kJ/mol	Joback Method
hfus	26.40	kJ/mol	Joback Method
hvap	66.22	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	1.939		Crippen Method
mcvol	116.540	ml/mol	McGowan Method
pc	5446.55	kPa	Joback Method
tb	663.85	K	Joback Method
tc	941.03	K	Joback Method
tf	495.51	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.58	J/mol×K	663.85	Joback Method
cpg	258.82	J/mol×K	710.05	Joback Method
cpg	266.30	J/mol×K	756.24	Joback Method
cpg	273.07	J/mol×K	802.44	Joback Method
cpg	279.20	J/mol×K	848.64	Joback Method
cpg	284.75	J/mol×K	894.83	Joback Method
cpg	289.78	J/mol×K	941.03	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C53324382&Units=SI

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