

2-Bromo-5-nitroaniline

Other names:	Benzenamine, 2-bromo-5-nitro-
Inchi:	InChI=1S/C6H5BrN2O2/c7-5-2-1-4(9(10)11)3-6(5)8/h1-3H,8H2
InchiKey:	BAAUCXCLMDAZEL-UHFFFAOYSA-N
Formula:	C6H5BrN2O2
SMILES:	<chem>Nc1cc([N+](=O)[O-])ccc1Br</chem>
Mol. weight [g/mol]:	217.02
CAS:	10403-47-1

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/molxK	663.85	Joback Method
cpg	258.82	J/molxK	710.05	Joback Method
cpg	266.30	J/molxK	756.24	Joback Method
cpg	273.07	J/molxK	802.44	Joback Method
cpg	279.20	J/molxK	848.64	Joback Method
cpg	284.75	J/molxK	894.83	Joback Method
cpg	289.78	J/molxK	941.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10403471&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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