4-Bromo-2-methyl-6-nitroaniline

Other names: Benzenamine, 4-bromo-2-methyl-6-nitro-
Inchi: InChI=1S/C7H7BrN2O2/c1-4-2-5(8)3-6(7(4)9)10(11)12/h2-3H,9H2,1H3
InchiKey: ZXFVKFUXKFPUQJ-UHFFFAOYSA-N
Formula: C7H7BrN2O2
SMILES: Cc1cc(Br)cc([N+](=O)[O-])c1N
Mol. weight [g/mol]: 231.05
CAS: 77811-44-0

Physical Properties

Property code	Value	Unit	Source
gf	207.90	kJ/mol	Joback Method
hf	63.67	kJ/mol	Joback Method
hfus	28.60	kJ/mol	Joback Method
hvap	69.11	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.248		Crippen Method
mcvol	130.630	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
tb	691.71	K	Joback Method
tc	962.68	K	Joback Method
tf	519.30	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.35	J/mol×K	691.71	Joback Method
cpg	304.48	J/mol×K	736.87	Joback Method
cpg	312.84	J/mol×K	782.03	Joback Method
cpg	320.50	J/mol×K	827.20	Joback Method
cpg	327.49	J/mol×K	872.36	Joback Method
cpg	333.87	J/mol×K	917.52	Joback Method
cpg	339.68	J/mol×K	962.68	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=C77811440&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume