Benzenamine, 4-bromo-3-methyl-

Other names:	5-Amino-2-bromotoluene
	4-Bromo-3-methylaniline
	4-Bromo-3-methylbenzenamine
	4-Bromo-m-toluidine
	3-Methyl-4-bromoaniline
	m-Toluidine, 4-bromo-
Inchi:	InChI=1S/C7H8BrN/c1-5-4-6(9)2-3-7(5)8/h2-4H,9H2,1H3
InchiKey:	MMEGELSFOYDPQW-UHFFFAOYSA-N
Formula:	C7H8BrN
SMILES:	Cc1cc(N)ccc1Br
Mol. weight [g/mol]:	186.05
CAS:	6933-10-4

Physical Properties

Property code	Value	Unit	Source
gf	181.98	kJ/mol	Joback Method
hf	85.90	kJ/mol	Joback Method
hfus	17.63	kJ/mol	Joback Method
hvap	51.85	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.340		Crippen Method
mcvol	113.210	ml/mol	McGowan Method
pc	4672.09	kPa	Joback Method
tb	513.20	K	NIST Webbook
tc	781.07	K	Joback Method
tf	363.17	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.00	J/mol×K	534.89	Joback Method
cpg	230.14	J/mol×K	575.92	Joback Method
cpg	239.59	J/mol×K	616.95	Joback Method

cpg	248.36	J/mol×K	657.98	Joback Method
cpg	256.52	J/mol×K	699.01	Joback Method
cpg	264.09	J/mol×K	740.04	Joback Method
cpg	271.11	J/mol×K	781.07	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=C6933104&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

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