

# Benzenamine, 3-bromo-4-methyl-

<b>Other names:</b>	p-Toluidine, 3-bromo- 3-Bromo-p-toluidine 3-Bromo-4-methylaniline 3-Bromo-1,4-toluidine 3-Bromo-4-methyl-phenylamine
<b>Inchi:</b>	InChI=1S/C7H8BrN/c1-5-2-3-6(9)4-7(5)8/h2-4H,9H2,1H3
<b>InchiKey:</b>	GRXMMIBZRMKADT-UHFFFAOYSA-N
<b>Formula:</b>	C7H8BrN
<b>SMILES:</b>	Cc1ccc(N)cc1Br
<b>Mol. weight [g/mol]:</b>	186.05
<b>CAS:</b>	7745-91-7

## 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	528.70	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/molxK	534.89	Joback Method
cpg	230.14	J/molxK	575.92	Joback Method
cpg	239.59	J/molxK	616.95	Joback Method
cpg	248.36	J/molxK	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

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C7745917&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7745917&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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