

# 3-Bromo-2,4,6-trimethylaniline

<b>Inchi:</b>	InChI=1S/C9H12BrN/c1-5-4-6(2)9(11)7(3)8(5)10/h4H,11H2,1-3H3
<b>InchiKey:</b>	MVLMPTBHZPYDBZ-UHFFFAOYSA-N
<b>Formula:</b>	C9H12BrN
<b>SMILES:</b>	Cc1cc(C)c(Br)c(C)c1N
<b>Mol. weight [g/mol]:</b>	214.10
<b>CAS:</b>	82842-52-2

## Physical Properties

Property code	Value	Unit	Source
gf	179.56	kJ/mol	Joback Method
hf	21.68	kJ/mol	Joback Method
hfus	22.03	kJ/mol	Joback Method
hvap	57.63	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.957		Crippen Method
mcvol	141.390	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
tb	590.61	K	Joback Method
tc	828.88	K	Joback Method
tf	410.75	K	Joback Method
vc	0.522	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.80	J/molxK	590.61	Joback Method
cpg	317.61	J/molxK	630.32	Joback Method
cpg	328.73	J/molxK	670.03	Joback Method
cpg	339.19	J/molxK	709.74	Joback Method
cpg	349.02	J/molxK	749.46	Joback Method
cpg	358.24	J/molxK	789.17	Joback Method
cpg	366.87	J/molxK	828.88	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=C82842522&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C82842522&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>mccvol:</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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