

# 2-Bromo-4-isopropylaniline

<b>Inchi:</b>	InChI=1S/C9H12BrN/c1-6(2)7-3-4-9(11)8(10)5-7/h3-6H,11H2,1-2H3
<b>InchiKey:</b>	WEMDUNBELVTSRP-UHFFFAOYSA-N
<b>Formula:</b>	C9H12BrN
<b>SMILES:</b>	CC(C)c1ccc(N)c(Br)c1
<b>Mol. weight [g/mol]:</b>	214.10
<b>CAS:</b>	51605-97-1

## Physical Properties

Property code	Value	Unit	Source
gf	196.38	kJ/mol	Joback Method
hf	39.34	kJ/mol	Joback Method
hfus	19.29	kJ/mol	Joback Method
hvap	55.92	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.155		Crippen Method
mcvol	141.390	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
tb	580.21	K	Joback Method
tc	821.77	K	Joback Method
tf	370.71	K	Joback Method
vc	0.516	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.18	J/molxK	580.21	Joback Method
cpg	320.87	J/molxK	620.47	Joback Method
cpg	332.71	J/molxK	660.73	Joback Method
cpg	343.73	J/molxK	700.99	Joback Method
cpg	353.98	J/molxK	741.25	Joback Method
cpg	363.51	J/molxK	781.51	Joback Method
cpg	372.36	J/molxK	821.77	Joback Method

# Sources

<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=C51605971&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C51605971&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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