

# 3,5-Dibromo-4-methylaniline

<b>Inchi:</b>	InChI=1S/C7H7Br2N/c1-4-6(8)2-5(10)3-7(4)9/h2-3H,10H2,1H3
<b>InchiKey:</b>	AQZDIKCNODUMNY-UHFFFAOYSA-N
<b>Formula:</b>	C7H7Br2N
<b>SMILES:</b>	Cc1c(Br)cc(N)cc1Br
<b>Mol. weight [g/mol]:</b>	264.94
<b>CAS:</b>	13194-73-5

## Physical Properties

Property code	Value	Unit	Source
gf	186.67	kJ/mol	Joback Method
hf	100.76	kJ/mol	Joback Method
hfus	22.53	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.102		Crippen Method
mcvol	130.710	ml/mol	McGowan Method
pc	5037.07	kPa	Joback Method
tb	606.03	K	Joback Method
tc	867.57	K	Joback Method
tf	435.49	K	Joback Method
vc	0.472	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.17	J/molxK	606.03	Joback Method
cpg	255.96	J/molxK	649.62	Joback Method
cpg	264.10	J/molxK	693.21	Joback Method
cpg	271.62	J/molxK	736.80	Joback Method
cpg	278.58	J/molxK	780.39	Joback Method
cpg	285.03	J/molxK	823.98	Joback Method
cpg	291.02	J/molxK	867.57	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=C13194735&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13194735&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>h vap:</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>m cvol:</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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