

# 1,4-Benzenediamine, 2-methyl-

<b>Other names:</b>	Toluene-2,5-diamine 4-Amino-2-methylaniline C.I. 76042 2,5-Diaminotoluene 2-Methyl-1,4-benzenediamine 2-Methyl-p-phenylenediamine p-Toluenediamine p-Toluyldiamine Toluylene-2,5-diamine p,m-Tolylenediamine
<b>Inchi:</b>	InChI=1S/C7H10N2/c1-5-4-6(8)2-3-7(5)9/h2-4H,8-9H2,1H3
<b>InchiKey:</b>	OBCSAIDCZQSFQH-UHFFFAOYSA-N
<b>Formula:</b>	C7H10N2
<b>SMILES:</b>	Cc1cc(N)ccc1N
<b>Mol. weight [g/mol]:</b>	122.17
<b>CAS:</b>	95-70-5

## Physical Properties

Property code	Value	Unit	Source
gf	234.11	kJ/mol	Joback Method
hf	93.36	kJ/mol	Joback Method
hfus	17.54	kJ/mol	Joback Method
hvap	56.06	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	1.159		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	4596.38	kPa	Joback Method
tb	541.26	K	Joback Method
tc	781.39	K	Joback Method
tf	386.63	K	Joback Method
vc	0.378	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.29	J/mol×K	541.26	Joback Method
cpg	248.42	J/mol×K	581.28	Joback Method
cpg	258.84	J/mol×K	621.30	Joback Method
cpg	268.59	J/mol×K	661.32	Joback Method
cpg	277.69	J/mol×K	701.34	Joback Method
cpg	286.17	J/mol×K	741.37	Joback Method
cpg	294.05	J/mol×K	781.39	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=C95705&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C95705&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>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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