

# Benzenamine, 2-chloro-4-(methylsulfonyl)-

<b>Other names:</b>	Aniline, 2-chloro-4-(methylsulfonyl)- 1-Amino-2-chloro-4-methylsulfonylbenzene 2-Chloro-4-(methylsulfonyl)aniline 3-Chloro-4-aminophenylmethylsulfone 4-Amino-3-chlorophenyl methyl sulfone 4-Amino-3-chlorofenylomethylosulfon 4-Amino-3-chlorophenylmethylsulphone 2-chloro-4-mesylianiline
<b>Inchi:</b>	InChI=1S/C7H8ClNO2S/c1-12(10,11)5-2-3-7(9)6(8)4-5/h2-4H,9H2,1H3
<b>InchiKey:</b>	VLMRGLCBIFWPGL-UHFFFAOYSA-N
<b>Formula:</b>	C7H8ClNO2S
<b>SMILES:</b>	CS(=O)(=O)c1ccc(N)c(Cl)c1
<b>Mol. weight [g/mol]:</b>	205.66
<b>CAS:</b>	13244-35-4

## Physical Properties

Property code	Value	Unit	Source
gf	-312.81	kJ/mol	Joback Method
hf	-409.52	kJ/mol	Joback Method
hfus	27.92	kJ/mol	Joback Method
hvap	68.44	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.326		Crippen Method
mcvol	136.040	ml/mol	McGowan Method
pc	5001.51	kPa	Joback Method
tb	553.94	K	Joback Method
tc	779.33	K	Joback Method
tf	371.85	K	Joback Method
vc	0.523	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.72	J/molxK	553.94	Joback Method

cpg	295.57	J/mol×K	591.50	Joback Method
cpg	305.72	J/mol×K	629.07	Joback Method
cpg	315.19	J/mol×K	666.63	Joback Method
cpg	323.98	J/mol×K	704.20	Joback Method
cpg	332.07	J/mol×K	741.76	Joback Method
cpg	339.49	J/mol×K	779.33	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C13244354&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13244354&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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