

# Benzenamine, 2-chloro-n-(1',1'-dimethylpropyl)-

Inchi:	InChI=1S/C11H16ClN/c1-4-11(2,3)13-10-8-6-5-7-9(10)12/h5-8,13H,4H2,1-3H3
InchiKey:	GXOZTGIQRYMPAG-UHFFFAOYSA-N
Formula:	C11H16ClN
SMILES:	CCC(C)(C)Nc1ccccc1Cl
Mol. weight [g/mol]:	197.70

## Physical Properties

Property code	Value	Unit	Source
gf	224.82	kJ/mol	Joback Method
hf	-16.33	kJ/mol	Joback Method
hfus	19.78	kJ/mol	Joback Method
hvap	52.54	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.941		Crippen Method
mcvol	164.310	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
tb	567.11	K	Joback Method
tc	789.06	K	Joback Method
tf	337.67	K	Joback Method
vc	0.617	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.13	J/molxK	567.11	Joback Method
cpg	398.82	J/molxK	604.10	Joback Method
cpg	413.42	J/molxK	641.09	Joback Method
cpg	427.01	J/molxK	678.09	Joback Method
cpg	439.64	J/molxK	715.08	Joback Method
cpg	451.38	J/molxK	752.07	Joback Method
cpg	462.29	J/molxK	789.06	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009278&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009278&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>
<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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