

# E-(3-Chloro-2-methyl-allyl)-dimethyl- amine

**Inchi:** InChI=1S/C5H10ClN/c1-5(4-6)7(2)3/h4H,1-3H3/b5-4+  
**InchiKey:** QFLUQQCVYSBOGC-SNAWJCMRSA-N  
**Formula:** C5H10ClN  
**SMILES:** CC(=CCl)N(C)C  
**Mol. weight [g/mol]:** 119.59

## Physical Properties

Property code	Value	Unit	Source
gf	161.74	kJ/mol	Joback Method
hf	12.69	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	33.19	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.648		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
rinpol	871.30		NIST Webbook
rinpol	871.30		NIST Webbook
ripol	1050.70		NIST Webbook
tb	367.71	K	Joback Method
tc	552.03	K	Joback Method
tf	189.46	K	Joback Method
vc	0.363	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.10	J/molxK	367.71	Joback Method
cpg	172.39	J/molxK	398.43	Joback Method
cpg	182.11	J/molxK	429.15	Joback Method
cpg	191.31	J/molxK	459.87	Joback Method
cpg	200.00	J/molxK	490.59	Joback Method
cpg	208.20	J/molxK	521.31	Joback Method
cpg	215.95	J/molxK	552.03	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=R153927&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R153927&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>ri<sub>npol</sub>:</b>	Non-polar retention indices
<b>ri<sub>pol</sub>:</b>	Polar retention indices
<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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