

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

<b>Inchi:</b>	InChI=1S/C13H26ClN/c1-4-6-8-10-15(13(3)12-14)11-9-7-5-2/h12H,4-11H2,1-3H3/b13-12
<b>InchiKey:</b>	RZTDCWHGMBEWKD-OUKQBFOZSA-N
<b>Formula:</b>	C13H26ClN
<b>SMILES:</b>	CCCCCN(CCCCC)C(C)=CCl
<b>Mol. weight [g/mol]:</b>	231.81

## Physical Properties

Property code	Value	Unit	Source
gf	229.10	kJ/mol	Joback Method
hf	-152.43	kJ/mol	Joback Method
hfus	35.54	kJ/mol	Joback Method
hvap	51.00	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.769		Crippen Method
mcvol	211.950	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
ripol	1503.40		NIST Webbook
ripol	1503.40		NIST Webbook
ripol	1628.60		NIST Webbook
ripol	1628.60		NIST Webbook
tb	550.75	K	Joback Method
tc	724.06	K	Joback Method
tf	279.62	K	Joback Method
vc	0.811	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.83	J/mol×K	550.75	Joback Method
cpg	528.12	J/mol×K	579.64	Joback Method
cpg	544.60	J/mol×K	608.52	Joback Method
cpg	560.29	J/mol×K	637.41	Joback Method
cpg	575.25	J/mol×K	666.29	Joback Method
cpg	589.49	J/mol×K	695.18	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=R153932&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R153932&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>

## 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>rinpol:</b>	Non-polar retention indices
<b>ripol:</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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