Z-(3-Chloro-2-methyl-allyl)-ethyl-methyl-amine

Inchi: InChI=1S/C7H14ClN/c1-4-9(3)6-7(2)5-8/h5H,4,6H2,1-3H3/b7-5-
InchiKey: BICIXFQYPOFIAB-ALCCZGGFSA-N
Formula: C7H14ClN
SMILES: CCN(C)CC(C)=CCl
Mol. weight [g/mol]: 147.65

Physical Properties

Property code	Value	Unit	Source
gf	178.58	kJ/mol	Joback Method
hf	-28.59	kJ/mol	Joback Method
hfus	20.00	kJ/mol	Joback Method
hvap	37.64	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	2.081		Crippen Method
mcvol	127.410	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	868.80		NIST Webbook
rinpol	868.80		NIST Webbook
ripol	1051.80		NIST Webbook
ripol	1051.80		NIST Webbook
tb	413.47	K	Joback Method
tc	595.76	K	Joback Method
tf	212.00	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.04	J/mol×K	413.47	Joback Method
cpg	249.74	J/mol×K	443.85	Joback Method
cpg	261.79	J/mol×K	474.23	Joback Method
cpg	273.22	J/mol×K	504.61	Joback Method
cpg	284.05	J/mol×K	534.99	Joback Method
cpg	294.31	J/mol×K	565.37	Joback Method

cpg	304.04	J/mol×K	595.76	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R154173&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume