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

Inchi: InChI=1S/C6H12ClN/c1-4-8(3)6(2)5-7/h5H,4H2,1-3H3/b6-5+
InchiKey: IDRWMSWDAZAIFQ-AATRIKPKSA-N
Formula: C6H12ClN
SMILES: CCN(C)C(C)=CCl
Mol. weight [g/mol]: 133.62

Physical Properties

Property code	Value	Unit	Source
gf	170.16	kJ/mol	Joback Method
hf	-7.95	kJ/mol	Joback Method
hfus	17.41	kJ/mol	Joback Method
hvap	35.42	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	2.038		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
rinpol	874.90		NIST Webbook
ripol	1052.50		NIST Webbook
tb	390.59	K	Joback Method
tc	574.04	K	Joback Method
tf	200.73	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.42	J/mol×K	390.59	Joback Method
cpg	209.98	J/mol×K	421.16	Joback Method
cpg	220.93	J/mol×K	451.74	Joback Method
cpg	231.30	J/mol×K	482.31	Joback Method
cpg	241.11	J/mol×K	512.89	Joback Method
cpg	250.40	J/mol×K	543.46	Joback Method
cpg	259.19	J/mol×K	574.04	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R153952&Units=SI

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