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

Inchi: InChI=1S/C5H10ClN/c1-3-7-5(2)4-6/h4,7H,3H2,1-2H3/b5-4+
InchiKey: RJJUPMSDHRVZJH-SNAWJCMRSA-N
Formula: C5H10ClN
SMILES: CCNC(C)=CCl
Mol. weight [g/mol]: 119.59

Physical Properties

Property code	Value	Unit	Source
gf	140.35	kJ/mol	Joback Method
hf	-1.37	kJ/mol	Joback Method
hfus	16.89	kJ/mol	Joback Method
hvap	37.58	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.696		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
rinpol	934.50		NIST Webbook
rinpol	934.50		NIST Webbook
ripol	1226.60		NIST Webbook
tb	405.44	K	Joback Method
tc	596.84	K	Joback Method
tf	209.65	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.51	J/mol×K	405.44	Joback Method
cpg	183.22	J/mol×K	437.34	Joback Method
cpg	192.41	J/mol×K	469.24	Joback Method
cpg	201.12	J/mol×K	501.14	Joback Method
cpg	209.37	J/mol×K	533.04	Joback Method
cpg	217.18	J/mol×K	564.94	Joback Method
cpg	224.57	J/mol×K	596.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R153947&Units=SI
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

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