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

Inchi: InChI=1S/C6H12ClN/c1-3-8-5-6(2)4-7/h4,8H,3,5H2,1-2H3/b6-4-
InchiKey: QTIDSXIXLKYRNP-XQRVVYSFSA-N
Formula: C6H12ClN
SMILES: CCNCC(C)=CCl
Mol. weight [g/mol]: 133.62

Physical Properties

Property code	Value	Unit	Source
gf	148.77	kJ/mol	Joback Method
hf	-22.01	kJ/mol	Joback Method
hfus	19.48	kJ/mol	Joback Method
hvap	39.81	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.739		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	954.70		NIST Webbook
rinpol	954.70		NIST Webbook
ripol	1262.90		NIST Webbook
ripol	1262.90		NIST Webbook
tb	428.32	K	Joback Method
tc	618.09	K	Joback Method
tf	220.92	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.26	J/mol×K	428.32	Joback Method
cpg	222.22	J/mol×K	459.95	Joback Method
cpg	232.62	J/mol×K	491.58	Joback Method
cpg	242.49	J/mol×K	523.21	Joback Method
cpg	251.84	J/mol×K	554.83	Joback Method
cpg	260.70	J/mol×K	586.46	Joback Method

cpg	269.11	J/mol×K	618.09	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=R154168&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