

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

Inchi: InChI=1S/C6H12CIN/c1-6(4-7)5-8(2)3/h4H,5H2,1-3H3/b6-4-
InchiKey: OEADZERSOZSOBG-XQRVVYSFSA-N
Formula: C6H12CIN
SMILES: CC(=CCI)CN(C)C
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	-1.41		Crippen Method
logp	1.691		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
rinpol	866.60		NIST Webbook
rinpol	866.60		NIST Webbook
ripol	1048.20		NIST Webbook
ripol	1048.20		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/molxK	390.59	Joback Method
cpg	209.98	J/molxK	421.16	Joback Method
cpg	220.93	J/molxK	451.74	Joback Method
cpg	231.30	J/molxK	482.31	Joback Method
cpg	241.11	J/molxK	512.89	Joback Method
cpg	250.40	J/molxK	543.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R154148&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

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