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

Inchi: InChI=1S/C8H16ClN/c1-4-10(5-2)7-8(3)6-9/h6H,4-5,7H2,1-3H3/b8-6-
InchiKey: BVXJEWUABPPPQF-VURMDHGXSA-N
Formula: C8H16ClN
SMILES: CCN(CC)CC(C)=CCl
Mol. weight [g/mol]: 161.67

Physical Properties

Property code	Value	Unit	Source
gf	187.00	kJ/mol	Joback Method
hf	-49.23	kJ/mol	Joback Method
hfus	22.59	kJ/mol	Joback Method
hvap	39.87	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.471		Crippen Method
mcvol	141.500	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	1022.20		NIST Webbook
ripol	1154.10		NIST Webbook
tb	436.35	K	Joback Method
tc	617.26	K	Joback Method
tf	223.27	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.84	J/mol×K	436.35	Joback Method
cpg	291.56	J/mol×K	466.50	Joback Method
cpg	304.59	J/mol×K	496.65	Joback Method
cpg	316.96	J/mol×K	526.81	Joback Method
cpg	328.71	J/mol×K	556.96	Joback Method
cpg	339.85	J/mol×K	587.11	Joback Method
cpg	350.41	J/mol×K	617.26	Joback Method

Sources

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=R154133&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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