

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

Inchi:	InChI=1S/C14H28ClN/c1-4-6-8-10-16(11-9-7-5-2)13-14(3)12-15/h12H,4-11,13H2,1-3H3/
InchiKey:	LBFSKUKLJZLKTD-OWBHPGMISA-N
Formula:	C14H28ClN
SMILES:	CCCCCN(CCCCC)CC(C)=CCl
Mol. weight [g/mol]:	245.83

Physical Properties

Property code	Value	Unit	Source
gf	237.52	kJ/mol	Joback Method
hf	-173.07	kJ/mol	Joback Method
hfus	38.13	kJ/mol	Joback Method
hvap	53.22	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.811		Crippen Method
mcvol	226.040	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
ripol	1525.20		NIST Webbook
ripol	1525.20		NIST Webbook
ripol	1651.30		NIST Webbook
ripol	1651.30		NIST Webbook
tb	573.63	K	Joback Method
tc	745.71	K	Joback Method
tf	290.89	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.53	J/molxK	573.63	Joback Method
cpg	580.30	J/molxK	602.31	Joback Method
cpg	597.24	J/molxK	630.99	Joback Method
cpg	613.39	J/molxK	659.67	Joback Method
cpg	628.78	J/molxK	688.35	Joback Method
cpg	643.45	J/molxK	717.03	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=R154153&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
mccvol:	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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