

Z-(3-chloro-2-methyl-allyl)-dibutyl-amine

Inchi:	InChI=1S/C12H24ClN/c1-4-6-8-14(9-7-5-2)11-12(3)10-13/h10H,4-9,11H2,1-3H3/b12-10-
InchiKey:	FLCIITYVSWLZFG-BENRWUELSA-N
Formula:	C12H24ClN
SMILES:	CCCCN(CCCC)CC(C)=CCl
Mol. weight [g/mol]:	217.78

Physical Properties

Property code	Value	Unit	Source
gf	220.68	kJ/mol	Joback Method
hf	-131.79	kJ/mol	Joback Method
hfus	32.95	kJ/mol	Joback Method
hvap	48.77	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	4.031		Crippen Method
mcvol	197.860	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	1364.20		NIST Webbook
rinpol	1364.20		NIST Webbook
ripol	1487.40		NIST Webbook
tb	527.87	K	Joback Method
tc	702.59	K	Joback Method
tf	268.35	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.71	J/molxK	527.87	Joback Method
cpg	477.46	J/molxK	556.99	Joback Method
cpg	493.40	J/molxK	586.11	Joback Method
cpg	508.59	J/molxK	615.23	Joback Method
cpg	523.05	J/molxK	644.35	Joback Method
cpg	536.82	J/molxK	673.47	Joback Method
cpg	549.93	J/molxK	702.59	Joback Method

Sources

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=R154128&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
ri_{npol}:	Non-polar retention indices
ri_{pol}:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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