

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

Inchi:	InChI=1S/C11H22ClN/c1-4-6-8-13(9-7-5-2)11(3)10-12/h10H,4-9H2,1-3H3/b11-10+
InchiKey:	ZZIWHDLPHPYLFH-ZHACJKMWSA-N
Formula:	C11H22ClN
SMILES:	CCCCN(CCCC)C(C)=CCl
Mol. weight [g/mol]:	203.75

Physical Properties

Property code	Value	Unit	Source
gf	212.26	kJ/mol	Joback Method
hf	-111.15	kJ/mol	Joback Method
hfus	30.36	kJ/mol	Joback Method
hvap	46.55	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.989		Crippen Method
mcvol	183.770	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	1362.80		NIST Webbook
rinpol	1362.80		NIST Webbook
ripol	1487.40		NIST Webbook
ripol	1487.40		NIST Webbook
tb	504.99	K	Joback Method
tc	681.23	K	Joback Method
tf	257.08	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.25	J/molxK	504.99	Joback Method
cpg	428.38	J/molxK	534.36	Joback Method
cpg	443.73	J/molxK	563.74	Joback Method
cpg	458.34	J/molxK	593.11	Joback Method
cpg	472.24	J/molxK	622.48	Joback Method
cpg	485.47	J/molxK	651.86	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=R153907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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