L-Leucine, N-methyl-N-(3-chloropropoxycarbonyl)-, 3-chloropropyl ester

Inchi: InChI=1S/C14H25Cl2NO4/c1-11(2)10-12(13(18)20-8-4-6-15)17(3)14(19)21-9-5-7-16/h11
InchiKey: MEZUTZGCLKKPRY-GFCCVEGCSA-N
Formula: C14H25Cl2NO4
SMILES: CC(C)CC(C(=O)OCCCCl)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 342.26

Physical Properties

Property code	Value	Unit	Source
gf	-318.80	kJ/mol	Joback Method
hf	-796.40	kJ/mol	Joback Method
hfus	41.96	kJ/mol	Joback Method
hvap	75.11	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.271		Crippen Method
mcvol	257.460	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	2173.00		NIST Webbook
rinpol	2173.00		NIST Webbook
tb	758.72	K	Joback Method
tc	947.78	K	Joback Method
tf	454.17	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.00	J/mol×K	758.72	Joback Method
cpg	737.50	J/mol×K	790.23	Joback Method
cpg	751.11	J/mol×K	821.74	Joback Method
cpg	763.86	J/mol×K	853.25	Joback Method
cpg	775.76	J/mol×K	884.76	Joback Method
cpg	786.82	J/mol×K	916.27	Joback Method
cpg	797.07	J/mol×K	947.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392408&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume