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

Inchi: InChI=1S/C17H32ClNO4/c1-13(2)8-6-10-22-16(20)15(12-14(3)4)19(5)17(21)23-11-7-9-1

InchiKey: QGCZEHTXFJPSPR-OAHLLOKOSA-N

Formula: C17H32ClNO4

SMILES: CC(C)CCCOC(=O)C(CC(C)C)N(C)C(=O)OCCCCl

Mol. weight [g/mol]: 349.89

Physical Properties

Property code	Value	Unit	Source
gf	-284.05	kJ/mol	Joback Method
hf	-847.86	kJ/mol	Joback Method
hfus	42.01	kJ/mol	Joback Method
hvap	77.01	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	4.078		Crippen Method
mcvol	287.490	ml/mol	McGowan Method
pc	1300.47	kPa	Joback Method
rinpol	2138.00		NIST Webbook
rinpol	2138.00		NIST Webbook
tb	789.49	K	Joback Method
tc	977.01	K	Joback Method
tf	443.06	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.08	J/mol×K	789.49	Joback Method
cpg	882.74	J/mol×K	820.74	Joback Method
cpg	898.38	J/mol×K	852.00	Joback Method
cpg	913.03	J/mol×K	883.25	Joback Method
cpg	926.71	J/mol×K	914.51	Joback Method
cpg	939.44	J/mol×K	945.76	Joback Method
cpg	951.23	J/mol×K	977.01	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392409&Units=SI

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