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

Inchi: InChI=1S/C16H30ClNO4/c1-5-6-7-10-21-15(19)14(12-13(2)3)18(4)16(20)22-11-8-9-17/h
InchiKey: QBCWQBFXNKWWSI-CQSZACIVSA-N
Formula: C16H30ClNO4
SMILES: CCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 335.87

Physical Properties

Property code	Value	Unit	Source
gf	-290.03	kJ/mol	Joback Method
hf	-821.94	kJ/mol	Joback Method
hfus	42.94	kJ/mol	Joback Method
hvap	75.17	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.832		Crippen Method
mcvol	273.400	ml/mol	McGowan Method
pc	1387.11	kPa	Joback Method
rinpol	2079.00		NIST Webbook
rinpol	2079.00		NIST Webbook
tb	767.05	K	Joback Method
tc	951.96	K	Joback Method
tf	446.79	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.42	J/mol×K	767.05	Joback Method
cpg	823.60	J/mol×K	797.87	Joback Method
cpg	838.84	J/mol×K	828.69	Joback Method
cpg	853.15	J/mol×K	859.50	Joback Method
cpg	866.56	J/mol×K	890.32	Joback Method
cpg	879.08	J/mol×K	921.14	Joback Method
cpg	890.73	J/mol×K	951.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392401&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

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