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

Inchi: InChI=1S/C29H56ClNO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-34-28(32)2
InchiKey: LDMQPQRPSGMBSK-HHHXNRCGSA-N
Formula: C29H56ClNO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 518.21

Physical Properties

Property code	Value	Unit	Source
gf	-180.57	kJ/mol	Joback Method
hf	-1090.26	kJ/mol	Joback Method
hfus	76.61	kJ/mol	Joback Method
hvap	104.11	kJ/mol	Joback Method
log10ws	-9.26		Crippen Method
logp	8.903		Crippen Method
mcvol	456.570	ml/mol	McGowan Method
pc	646.48	kPa	Joback Method
rinpol	3409.00		NIST Webbook
tb	1064.49	K	Joback Method
tc	1335.56	K	Joback Method
tf	593.30	K	Joback Method
vc	1.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1614.22	J/mol×K	1064.49	Joback Method
cpg	1636.53	J/mol×K	1109.67	Joback Method
cpg	1656.41	J/mol×K	1154.85	Joback Method
cpg	1673.99	J/mol×K	1200.02	Joback Method
cpg	1689.42	J/mol×K	1245.20	Joback Method
cpg	1702.83	J/mol×K	1290.38	Joback Method
cpg	1714.37	J/mol×K	1335.56	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=U392407&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