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

Inchi: InChI=1S/C28H54ClNO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-33-27(31)26(2
Inchikey: CLKAWMODSXBRNK-AREMUKBSSA-N
Formula: C28H54ClNO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 504.19

Physical Properties

Property code	Value	Unit	Source
gf	-188.99	kJ/mol	Joback Method
hf	-1069.62	kJ/mol	Joback Method
hfus	74.02	kJ/mol	Joback Method
hvap	101.89	kJ/mol	Joback Method
log10ws	-8.84		Crippen Method
logp	8.513		Crippen Method
mcvol	442.480	ml/mol	McGowan Method
pc	679.23	kPa	Joback Method
rinpol	3312.00		NIST Webbook
rinpol	3312.00		NIST Webbook
tb	1041.61	K	Joback Method
tc	1298.77	K	Joback Method
tf	582.03	K	Joback Method
vc	1.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1549.48	J/mol×K	1041.61	Joback Method
cpg	1571.08	J/mol×K	1084.47	Joback Method
cpg	1590.48	J/mol×K	1127.33	Joback Method
cpg	1607.80	J/mol×K	1170.19	Joback Method
cpg	1623.13	J/mol×K	1213.05	Joback Method
cpg	1636.61	J/mol×K	1255.91	Joback Method
cpg	1648.33	J/mol×K	1298.77	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=U392406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume