l-Leucine, N-(5-chlorovaleryl)-, methyl ester

Inchi: InChI=1S/C12H22ClNO3/c1-9(2)8-10(12(16)17-3)14-11(15)6-4-5-7-13/h9-10H,4-8H2,1-3
InchiKey: DWVUQKRUDKYQKT-UHFFFAOYSA-N
Formula: C12H22ClNO3
SMILES: COC(=O)C(CC(C)C)NC(=O)CCCCCl
Mol. weight [g/mol]: 263.76

Physical Properties

Property code	Value	Unit	Source
gf	-240.10	kJ/mol	Joback Method
hf	-621.22	kJ/mol	Joback Method
hfus	33.47	kJ/mol	Joback Method
hvap	68.25	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.099		Crippen Method
mcvol	211.170	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	1796.00		NIST Webbook
rinpol	1796.00		NIST Webbook
tb	690.84	K	Joback Method
tc	880.76	K	Joback Method
tf	399.67	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.99	J/mol×K	690.84	Joback Method
cpg	588.21	J/mol×K	722.49	Joback Method
cpg	601.65	J/mol×K	754.15	Joback Method
cpg	614.33	J/mol×K	785.80	Joback Method
cpg	626.27	J/mol×K	817.45	Joback Method
cpg	637.46	J/mol×K	849.10	Joback Method
cpg	647.94	J/mol×K	880.76	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=U299716&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