L-Valine, N-(5-chlorovaleryl)-, isohexyl ester

Inchi: InChI=1S/C16H30ClNO3/c1-12(2)8-7-11-21-16(20)15(13(3)4)18-14(19)9-5-6-10-17/h12-
InchiKey: CFLOADQQRCJLEQ-UHFFFAOYSA-N
Formula: C16H30ClNO3
SMILES: CC(C)CCCOC(=O)C(NC(=O)CCCCCl)C(C)C
Mol. weight [g/mol]: 319.87

Physical Properties

Property code	Value	Unit	Source
gf	-208.86	kJ/mol	Joback Method
hf	-709.06	kJ/mol	Joback Method
hfus	40.31	kJ/mol	Joback Method
hvap	76.77	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.516		Crippen Method
mcvol	267.530	ml/mol	McGowan Method
pc	1429.38	kPa	Joback Method
rinpol	2188.00		NIST Webbook
rinpol	2188.00		NIST Webbook
tb	781.92	K	Joback Method
tc	972.17	K	Joback Method
tf	429.75	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.78	J/mol×K	781.92	Joback Method
cpg	812.74	J/mol×K	813.63	Joback Method
cpg	827.75	J/mol×K	845.34	Joback Method
cpg	841.83	J/mol×K	877.04	Joback Method
cpg	855.01	J/mol×K	908.75	Joback Method
cpg	867.30	J/mol×K	940.46	Joback Method
cpg	878.74	J/mol×K	972.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346586&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