l-Valine, N-(5-chlrovaleryl)-, methyl ester

Inchi: InChI=1S/C11H20ClNO3/c1-8(2)10(11(15)16-3)13-9(14)6-4-5-7-12/h8,10H,4-7H2,1-3H3
InchiKey: ZDCLUYAODLSBMX-UHFFFAOYSA-N
Formula: C11H20ClNO3
SMILES: COC(=O)C(NC(=O)CCCCCl)C(C)C
Mol. weight [g/mol]: 249.73

Physical Properties

Property code	Value	Unit	Source
gf	-248.52	kJ/mol	Joback Method
hf	-600.58	kJ/mol	Joback Method
hfus	30.88	kJ/mol	Joback Method
hvap	66.03	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.709		Crippen Method
mcvol	197.080	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
tb	667.96	K	Joback Method
tc	859.44	K	Joback Method
tf	388.40	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.39	J/mol×K	667.96	Joback Method
cpg	535.11	J/mol×K	699.87	Joback Method
cpg	548.09	J/mol×K	731.79	Joback Method
cpg	560.35	J/mol×K	763.70	Joback Method
cpg	571.88	J/mol×K	795.61	Joback Method
cpg	582.71	J/mol×K	827.53	Joback Method
cpg	592.85	J/mol×K	859.44	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=U299715&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