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

Inchi: InChI=1S/C14H26ClNO3/c1-10(2)9-19-14(18)13(11(3)4)16-12(17)7-5-6-8-15/h10-11,13H
InchiKey: HVHZIDOMBYAFJX-UHFFFAOYSA-N
Formula: C14H26ClNO3
SMILES: CC(C)COC(=O)C(NC(=O)CCCCCl)C(C)C
Mol. weight [g/mol]: 291.81

Physical Properties

Property code	Value	Unit	Source
gf	-225.70	kJ/mol	Joback Method
hf	-667.78	kJ/mol	Joback Method
hfus	35.13	kJ/mol	Joback Method
hvap	72.32	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.735		Crippen Method
mcvol	239.350	ml/mol	McGowan Method
pc	1661.90	kPa	Joback Method
rinpol	2012.00		NIST Webbook
rinpol	2012.00		NIST Webbook
tb	736.16	K	Joback Method
tc	926.66	K	Joback Method
tf	407.21	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.44	J/mol×K	736.16	Joback Method
cpg	698.72	J/mol×K	767.91	Joback Method
cpg	713.12	J/mol×K	799.66	Joback Method
cpg	726.65	J/mol×K	831.41	Joback Method
cpg	739.35	J/mol×K	863.16	Joback Method
cpg	751.23	J/mol×K	894.91	Joback Method
cpg	762.30	J/mol×K	926.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346583&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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