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

Inchi: InChI=1S/C15H28ClNO3/c1-4-5-8-11-20-15(19)14(12(2)3)17-13(18)9-6-7-10-16/h12,14H
InchiKey: XHDWNENBSOXOHU-UHFFFAOYSA-N
Formula: C15H28ClNO3
SMILES: CCCCCOC(=O)C(NC(=O)CCCCCl)C(C)C
Mol. weight [g/mol]: 305.84

Physical Properties

Property code	Value	Unit	Source
gf	-214.84	kJ/mol	Joback Method
hf	-683.14	kJ/mol	Joback Method
hfus	41.24	kJ/mol	Joback Method
hvap	74.93	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.270		Crippen Method
mcvol	253.440	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	2148.00		NIST Webbook
rinpol	2148.00		NIST Webbook
tb	759.48	K	Joback Method
tc	947.48	K	Joback Method
tf	433.48	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.07	J/mol×K	759.48	Joback Method
cpg	754.52	J/mol×K	790.81	Joback Method
cpg	769.09	J/mol×K	822.15	Joback Method
cpg	782.78	J/mol×K	853.48	Joback Method
cpg	795.64	J/mol×K	884.81	Joback Method
cpg	807.67	J/mol×K	916.15	Joback Method
cpg	818.89	J/mol×K	947.48	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=U346585&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