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

Inchi: InChI=1S/C19H36ClNO3/c1-4-5-6-7-8-9-12-15-24-19(23)18(16(2)3)21-17(22)13-10-11-1
InchiKey: PHYKVLYJPOAMRG-UHFFFAOYSA-N
Formula: C19H36ClNO3
SMILES: CCCCCCCCCOC(=O)C(N=C(O)CCCCCl)C(C)C
Mol. weight [g/mol]: 361.95

Physical Properties

Property code	Value	Unit	Source
hf	-786.39	kJ/mol	Joback Method
hvap	90.73	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	5.670		Crippen Method
mcvol	309.800	ml/mol	McGowan Method
pc	1092.82	kPa	Joback Method
rinpol	2545.00		NIST Webbook
rinpol	2545.00		NIST Webbook
tb	915.70	K	Joback Method
tc	1121.10	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346587&Units=SI

Legend

hf: Enthalpy of formation 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