D-Alanine, N-(5-chlorovaleryl)-, isohexyl ester

Inchi: InChI=1S/C14H26ClNO3/c1-11(2)7-6-10-19-14(18)12(3)16-13(17)8-4-5-9-15/h11-12H,4-
InchiKey: GNZLWQRTBQAPBZ-UHFFFAOYSA-N
Formula: C14H26ClNO3
SMILES: CC(C)CCCOC(=O)C(C)NC(=O)CCCCCl
Mol. weight [g/mol]: 291.81

Physical Properties

Property code	Value	Unit	Source
gf	-223.26	kJ/mol	Joback Method
hf	-662.50	kJ/mol	Joback Method
hfus	38.65	kJ/mol	Joback Method
hvap	72.70	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.880		Crippen Method
mcvol	239.350	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	2103.00		NIST Webbook
tb	736.60	K	Joback Method
tc	924.73	K	Joback Method
tf	422.21	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.91	J/mol×K	736.60	Joback Method
cpg	697.99	J/mol×K	767.95	Joback Method
cpg	712.21	J/mol×K	799.31	Joback Method
cpg	725.61	J/mol×K	830.66	Joback Method
cpg	738.19	J/mol×K	862.02	Joback Method
cpg	749.98	J/mol×K	893.37	Joback Method
cpg	760.99	J/mol×K	924.73	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=U348481&Units=SI

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