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

Inchi: InChI=1S/C14H26ClNO3/c1-3-4-5-8-11-19-14(18)12(2)16-13(17)9-6-7-10-15/h12H,3-11H
InchiKey: JAYPLEGBRSWVSE-UHFFFAOYSA-N
Formula: C14H26ClNO3
SMILES: CCCCCCOC(=O)C(C)NC(=O)CCCCCl
Mol. weight [g/mol]: 291.81

Physical Properties

Property code	Value	Unit	Source
gf	-220.82	kJ/mol	Joback Method
hf	-657.22	kJ/mol	Joback Method
hfus	42.17	kJ/mol	Joback Method
hvap	73.09	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.024		Crippen Method
mcvol	239.350	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	2146.00		NIST Webbook
rinpol	2146.00		NIST Webbook
tb	737.04	K	Joback Method
tc	922.94	K	Joback Method
tf	437.21	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.39	J/mol×K	737.04	Joback Method
cpg	697.27	J/mol×K	768.02	Joback Method
cpg	711.33	J/mol×K	799.01	Joback Method
cpg	724.58	J/mol×K	829.99	Joback Method
cpg	737.06	J/mol×K	860.97	Joback Method
cpg	748.76	J/mol×K	891.95	Joback Method
cpg	759.72	J/mol×K	922.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348482&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